



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 02:43 PM EDT

PDB ID : 6W1Q / pdb_00006w1q
Title : RT XFEL structure of Photosystem II 50 microseconds after the second illumination at 2.27 Angstrom resolution
Authors : Ibrahim, M.; Fransson, T.; Chatterjee, R.; Cheah, M.H.; Hussein, R.; Lassalle, L.; Sutherlin, K.D.; Young, I.D.; Fuller, F.D.; Gul, S.; Kim, I.-S.; Simon, P.S.; de Lichtenberg, C.; Chernev, P.; Bogacz, I.; Pham, C.; Orville, A.M.; Saichek, N.; Northen, T.R.; Batyuk, A.; Carbajo, S.; Alonso-Mori, R.; Tono, K.; Owada, S.; Bhowmick, A.; Bolotovskii, R.; Mendez, D.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Brewster, A.S.; Adams, P.D.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2020-03-04
Resolution : 2.27 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	: 4-5-2 with Phenix2.0
Mogul	: 2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	: 2.0
EDS	: 3.0
Buster-report	: wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	: 20250101.v01 (using entries in the PDB archive January 1st 2025)

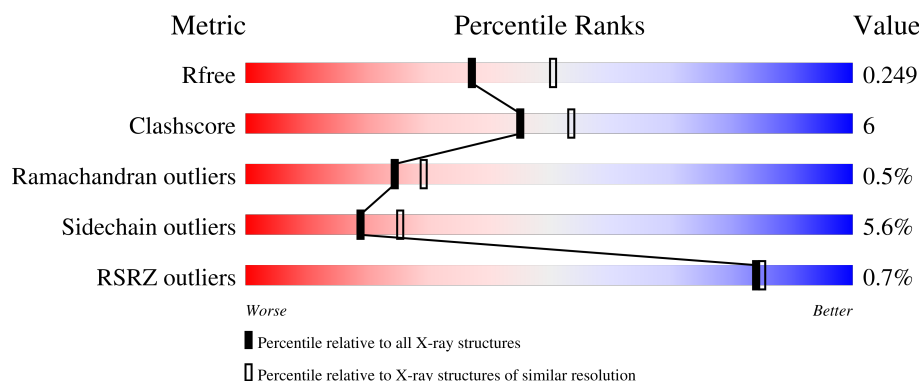
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

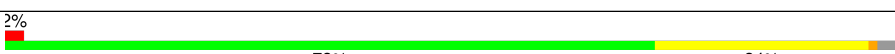
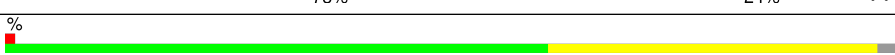
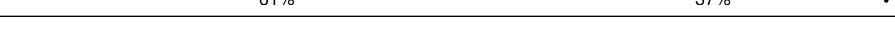
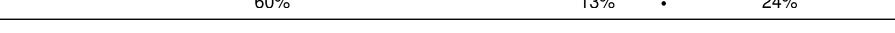
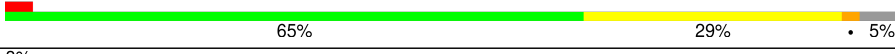
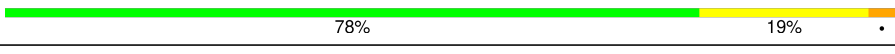
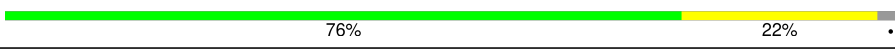
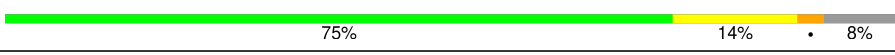
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	

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CCP4 : 9.0.015 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.50

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Mol	Chain	Length	Quality of chain
2	B	506	
2	b	506	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	R	41	

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Mol	Chain	Length	Quality of chain
14	r	41	
15	T	30	
15	t	30	
16	U	134	
16	u	134	
17	V	163	
17	v	163	
18	X	41	
18	x	41	
19	Y	46	
19	y	46	
20	Z	62	
20	z	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	HEC	F	101	X	-	-	-
34	HEC	V	201	X	-	-	-
34	HEC	f	101	X	-	-	-
34	HEC	v	201	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 103197 atoms, of which 51556 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	0	0
			5130	1717	2508	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5118	1714	2499	431	459	15			

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7864	2631	3859	666	695	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7800	2610	3822	665	690	13			

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	2	0
			6767	2249	3341	571	593	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6913	2290	3413	587	610	13			

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	0	0
			5330	1800	2613	444	461	12			
4	d	341	Total	C	H	N	O	S	0	1	0
			5342	1804	2619	444	463	12			

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	H	N	O	0	1	0
			1316	436	650	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	108	122			

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	H	N	O	0	0	0
			556	187	281	45	42			
6	f	34	Total	C	H	N	O	0	0	0
			556	187	281	45	42			

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	H	N	O	0	0	0
			1042	341	532	82	85			
7	h	63	Total	C	H	N	O	0	0	0
			1016	333	518	80	83			

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			
8	i	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	initiating methionine	UNP Q8DJZ6
i	1	FME	-	initiating methionine	UNP Q8DJZ6

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	H	N	O	0	0	0
			525	174	268	40	42			
9	j	36	Total	C	H	N	O	0	0	0
			525	174	268	40	42			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	H	N	O	0	0	0
			620	202	316	48	53			
11	l	36	Total	C	H	N	O	0	0	0
			600	197	304	47	52			

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	H	N	O	0	0	0
			525	171	269	37	47			
12	m	32	Total	C	H	N	O	0	0	0
			518	168	267	36	46			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	initiating methionine	UNP Q8DHA7
m	1	FME	-	initiating methionine	UNP Q8DHA7

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	0	1	0
			3698	1168	1828	313	385			
13	o	244	Total	C	H	N	O	0	0	0
			3718	1170	1844	317	383			

- Molecule 14 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	R	34	Total	C	H	N	O	0	0	0
			569	184	298	47	40			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	r	31	Total	C	H	N	O	0	0	0
			493	162	253	42	36			

- Molecule 15 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	30	Total	C	H	N	O	S	0	0
			519	181	261	36	39	2		
15	t	30	Total	C	H	N	O	S	0	0
			512	180	256	36	38	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	initiating methionine	UNP Q8DIQ0
t	1	FME	-	initiating methionine	UNP Q8DIQ0

- Molecule 16 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	U	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			
16	u	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			

- Molecule 17 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	V	137	Total	C	H	N	O	S	0	0
			2132	675	1068	177	208	4		
17	v	137	Total	C	H	N	O	S	0	0
			2132	675	1068	177	208	4		

- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			
18	x	39	Total	C	H	N	O	0	0	0
			602	191	316	46	49			

- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
19	Y	27	Total	C	H	N	O	S	0	0	0
			413	128	217	35	30	3			
19	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	35	36	3			

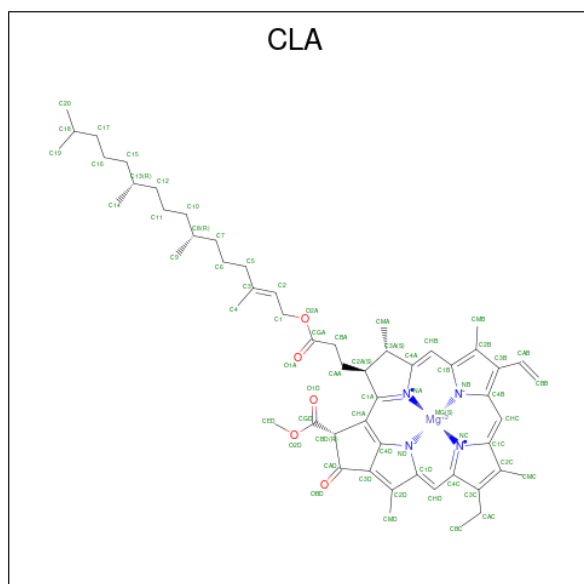
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
20	Z	62	Total 995	C 328	H 516	N 72	O 77	S 2	0	0	0
20	z	62	Total 986	C 326	H 509	N 72	O 77	S 2	0	0	0

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	0
			1	1		
21	a	1	Total	Fe	0	0
			1	1		

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	H	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

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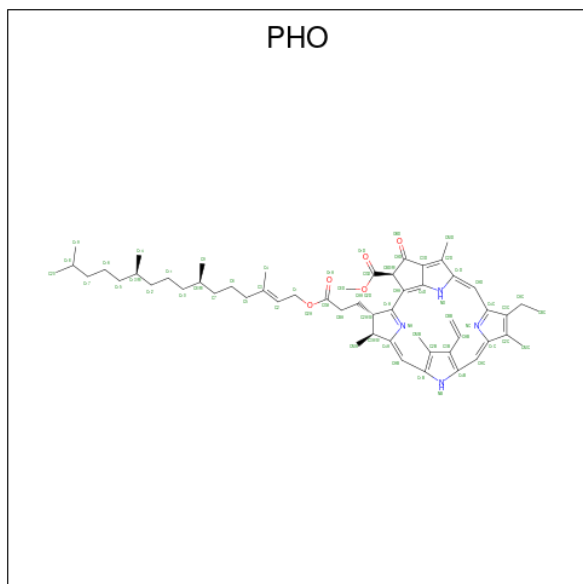
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			132	54	68	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

- Molecule 23 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).

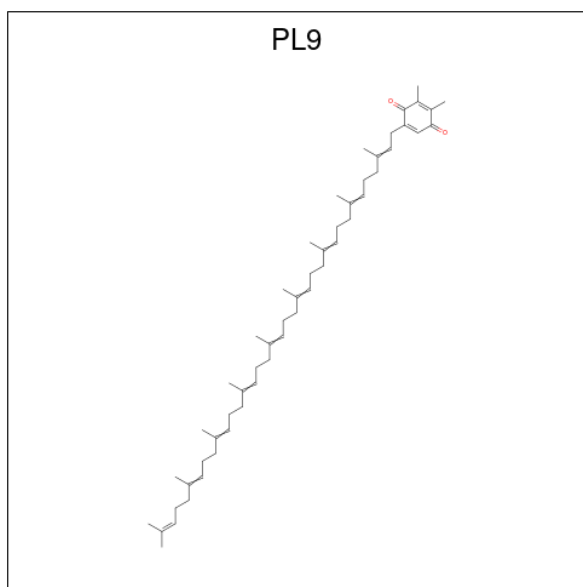


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

- Molecule 24 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

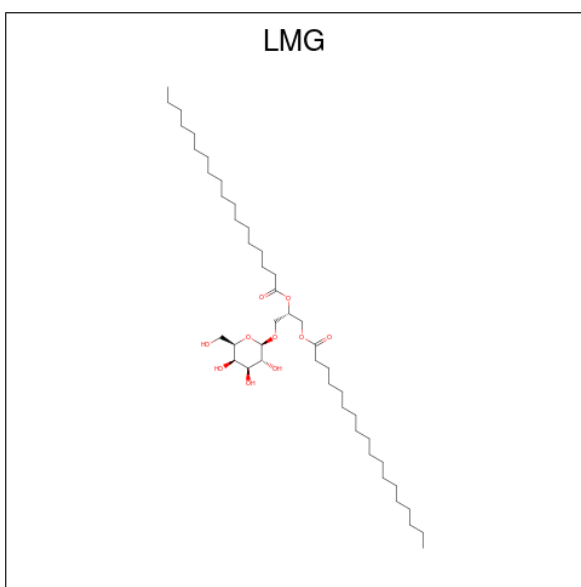
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	2	Total	Cl	0	0
			2	2		
24	a	2	Total	Cl	0	0
			2	2		

- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	H	O	0	0
			135	53	80	2		
25	D	1	Total	C	H	O	0	0
			135	53	80	2		
25	a	1	Total	C	H	O	0	0
			135	53	80	2		
25	d	1	Total	C	H	O	0	0
			135	53	80	2		

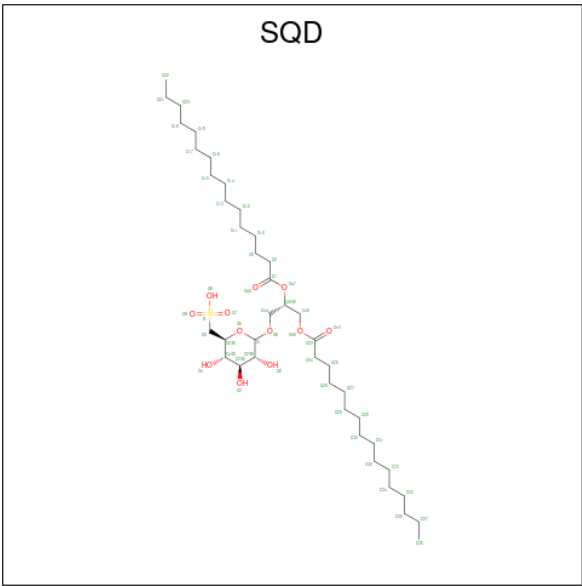
- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			114	38	66	10		
26	B	1	Total	C	H	O	0	0
			68	24	40	4		
26	D	1	Total	C	H	O	0	0
			120	41	69	10		
26	D	1	Total	C	H	O	0	0
			78	27	45	6		
26	M	1	Total	C	H	O	0	0
			120	41	69	10		
26	Y	1	Total	C	H	O	0	0
			114	38	66	10		
26	a	1	Total	C	H	O	0	0
			140	45	85	10		
26	b	1	Total	C	H	O	0	0
			141	45	86	10		
26	c	1	Total	C	H	O	0	0
			79	27	42	10		
26	c	1	Total	C	H	O	0	0
			116	38	68	10		
26	c	1	Total	C	H	O	0	0
			117	39	68	10		
26	d	1	Total	C	H	O	0	0
			101	34	57	10		
26	m	1	Total	C	H	O	0	0
			122	41	71	10		

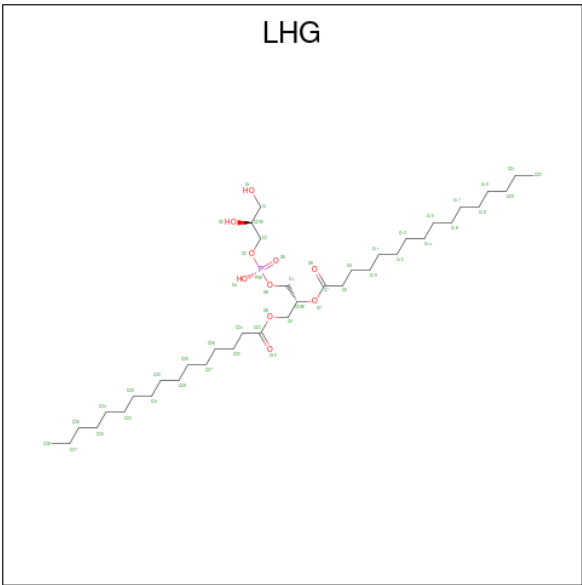
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



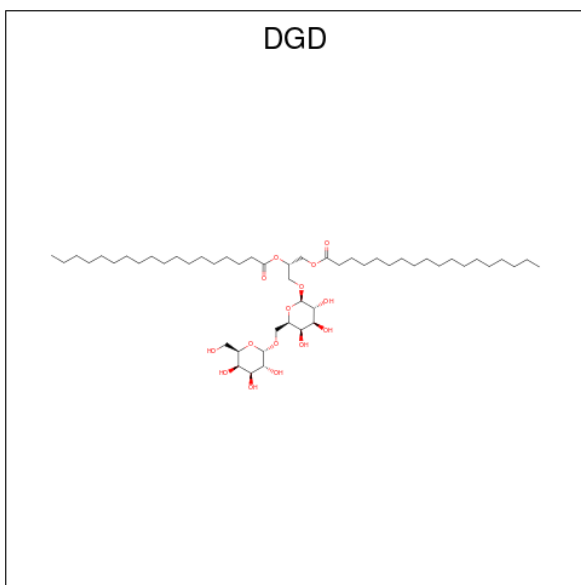
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	A	1	Total	C	H	O	S	0	0
			121	39	69	12	1		
27	A	1	Total	C	H	O		0	0
			104	35	65	4			
27	B	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
27	D	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
27	L	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
27	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
27	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		
27	t	1	Total	C	H	O		0	0
			92	31	56	5			

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



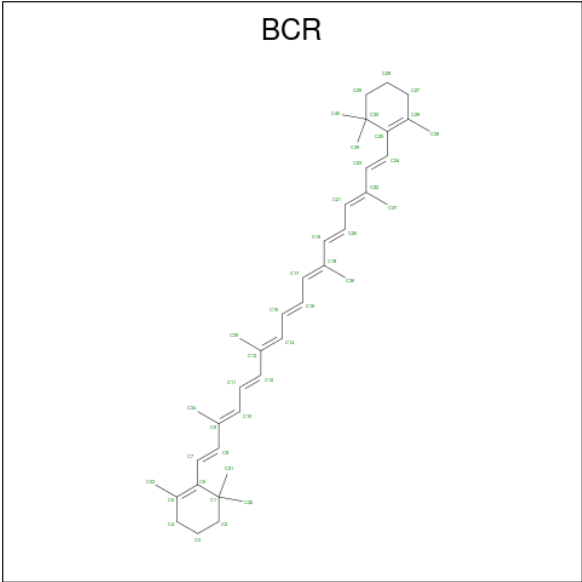
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	D	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	D	1	Total	C	H	O	P	0	0
			113	36	66	10	1		
28	D	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	L	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	a	1	Total	C	H	O	P	0	0
			97	31	55	10	1		
28	b	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	d	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	d	1	Total	C	H	O	P	0	0
			88	28	49	10	1		
28	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			160	51	94	15		
29	C	1	Total	C	H	O	0	0
			143	47	81	15		
29	C	1	Total	C	H	O	0	0
			143	47	81	15		
29	C	1	Total	C	H	O	0	0
			141	47	79	15		
29	H	1	Total	C	H	O	0	0
			139	47	77	15		
29	c	1	Total	C	H	O	0	0
			141	47	79	15		
29	c	1	Total	C	H	O	0	0
			140	47	78	15		
29	c	1	Total	C	H	O	0	0
			139	47	77	15		
29	h	1	Total	C	H	O	0	0
			141	47	79	15		

- Molecule 30 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



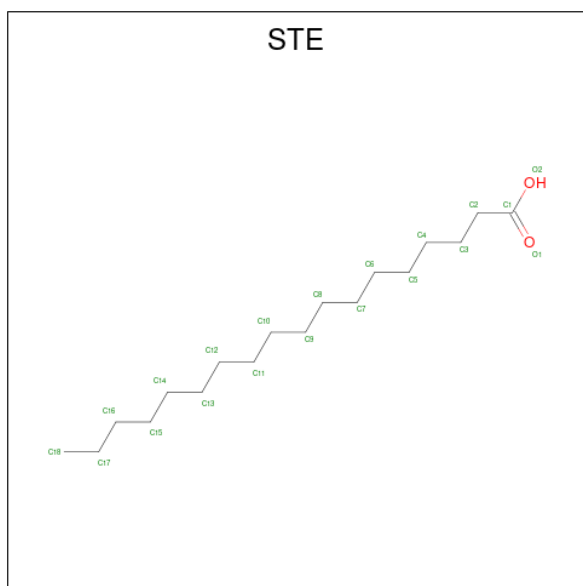
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	B	1	Total	C	H	0	0
			96	40	56		
30	B	1	Total	C	H	0	0
			96	40	56		
30	B	1	Total	C	H	0	0
			96	40	56		
30	C	1	Total	C	H	0	0
			96	40	56		
30	C	1	Total	C	H	0	0
			96	40	56		
30	D	1	Total	C	H	0	0
			96	40	56		
30	H	1	Total	C	H	0	0
			96	40	56		
30	I	1	Total	C	H	0	0
			96	40	56		
30	K	1	Total	C	H	0	0
			96	40	56		
30	K	1	Total	C	H	0	0
			96	40	56		
30	T	1	Total	C	H	0	0
			96	40	56		
30	a	1	Total	C	H	0	0
			96	40	56		
30	b	1	Total	C	H	0	0
			96	40	56		
30	b	1	Total	C	H	0	0
			96	40	56		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	b	1	Total	C	H	0	0
			96	40	56		
30	c	1	Total	C	H	0	0
			96	40	56		
30	d	1	Total	C	H	0	0
			96	40	56		
30	k	1	Total	C	H	0	0
			96	40	56		
30	k	1	Total	C	H	0	0
			96	40	56		
30	k	1	Total	C	H	0	0
			96	40	56		
30	t	1	Total	C	H	0	0
			96	40	56		
30	x	1	Total	C	H	0	0
			96	40	56		

- Molecule 31 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total	C	H	O	0	0
			43	15	26	2		
31	B	1	Total	C	H	O	0	0
			28	10	16	2		
31	B	1	Total	C	H	O	0	0
			46	16	28	2		

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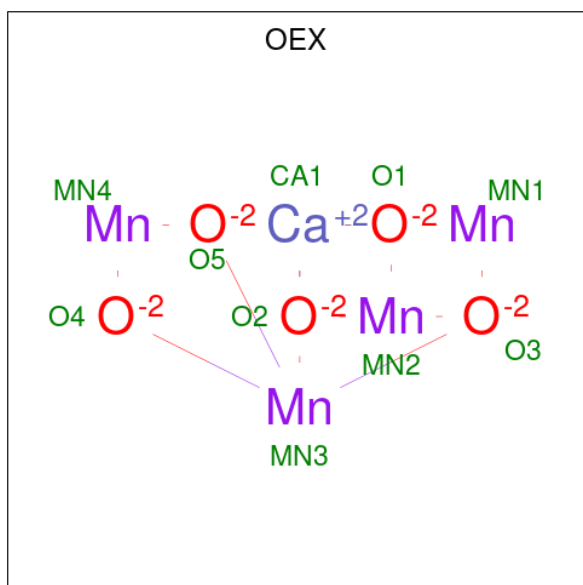
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	B	1	Total C H 47 16 31	0	0
31	B	1	Total C H O 28 10 16 2	0	0
31	C	1	Total C H O 28 10 16 2	0	0
31	C	1	Total C H 47 16 31	0	0
31	C	1	Total C H O 28 10 16 2	0	0
31	H	1	Total C H 53 18 35	0	0
31	I	1	Total C H 41 15 26	0	0
31	J	1	Total C H O 28 10 16 2	0	0
31	L	1	Total C H O 28 10 16 2	0	0
31	M	1	Total C H O 37 13 22 2	0	0
31	M	1	Total C H 26 10 16	0	0
31	M	1	Total C H 53 18 35	0	0
31	R	1	Total C H O 28 10 16 2	0	0
31	X	1	Total C H O 55 18 35 2	0	0
31	Z	1	Total C H 20 8 12	0	0
31	a	1	Total C H O 28 10 16 2	0	0
31	a	1	Total C H 41 15 26	0	0
31	b	1	Total C H 47 16 31	0	0
31	b	1	Total C H O 55 18 35 2	0	0
31	b	1	Total C H O 40 14 24 2	0	0
31	b	1	Total C H 44 15 29	0	0

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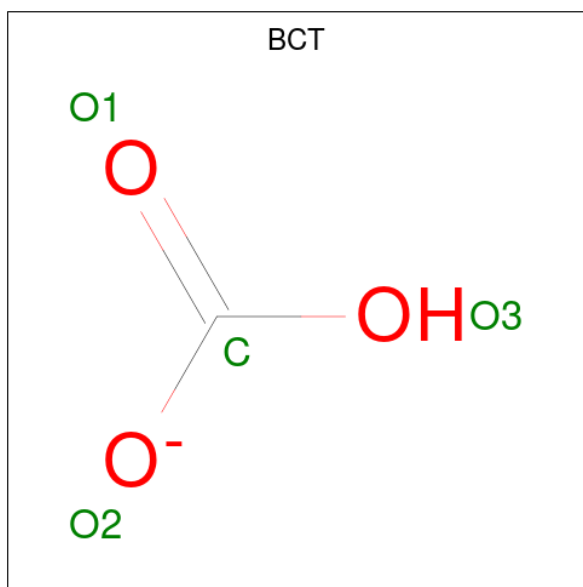
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	b	1	Total	C	H	O	0	0
			55	18	35	2		
31	b	1	Total	C	H		0	0
			26	10	16			
31	b	1	Total	C	H		0	0
			41	14	27			
31	b	1	Total	C	H	O	0	0
			55	18	35	2		
31	c	1	Total	C	H	O	0	0
			55	18	35	2		
31	d	1	Total	C	H	O	0	0
			43	15	26	2		
31	j	1	Total	C	H	O	0	0
			28	10	16	2		
31	k	1	Total	C	H	O	0	0
			28	10	16	2		
31	t	1	Total	C	H	O	0	0
			34	12	20	2		
31	t	1	Total	C	H		0	0
			26	10	16			
31	x	1	Total	C	H	O	0	0
			55	18	35	2		

- Molecule 32 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	C	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
32	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	D	1	Total	C	H	O	0	0
			5	1	1	3		
33	d	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 34 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	E	22	Total O 22 22	0	0
36	F	6	Total O 6 6	0	0
36	H	16	Total O 16 16	0	0
36	I	10	Total O 10 10	0	0
36	J	14	Total O 14 14	0	0
36	K	3	Total O 3 3	0	0
36	L	10	Total O 10 10	0	0
36	M	9	Total O 9 9	0	0
36	O	60	Total O 60 60	0	0
36	R	11	Total O 11 11	0	0
36	T	8	Total O 8 8	0	0
36	U	28	Total O 28 28	0	0
36	V	49	Total O 49 49	0	0
36	X	10	Total O 10 10	0	0
36	Y	2	Total O 2 2	0	0
36	Z	7	Total O 7 7	0	0
36	a	96	Total O 96 96	0	0
36	b	116	Total O 116 116	0	0
36	c	108	Total O 108 108	0	0
36	d	87	Total O 87 87	0	0
36	e	11	Total O 11 11	0	0

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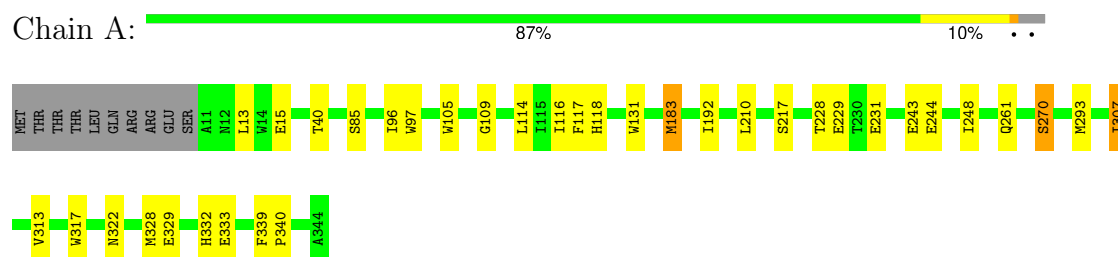
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	f	7	Total 7	O 7	0	0
36	h	17	Total 17	O 17	0	0
36	i	14	Total 14	O 14	0	0
36	j	8	Total 8	O 8	0	0
36	k	7	Total 7	O 7	0	0
36	l	11	Total 11	O 11	0	0
36	m	4	Total 4	O 4	0	0
36	o	67	Total 67	O 67	0	0
36	r	3	Total 3	O 3	0	0
36	t	8	Total 8	O 8	0	0
36	u	34	Total 34	O 34	0	0
36	v	30	Total 30	O 30	0	0
36	x	6	Total 6	O 6	0	0
36	y	12	Total 12	O 12	0	0
36	z	6	Total 6	O 6	0	0

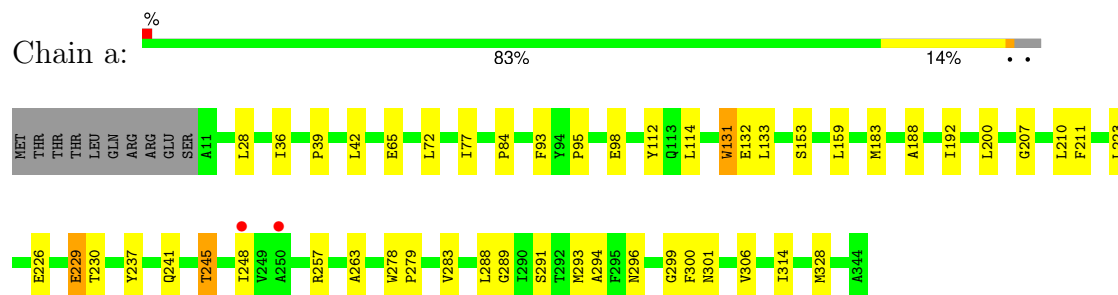
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

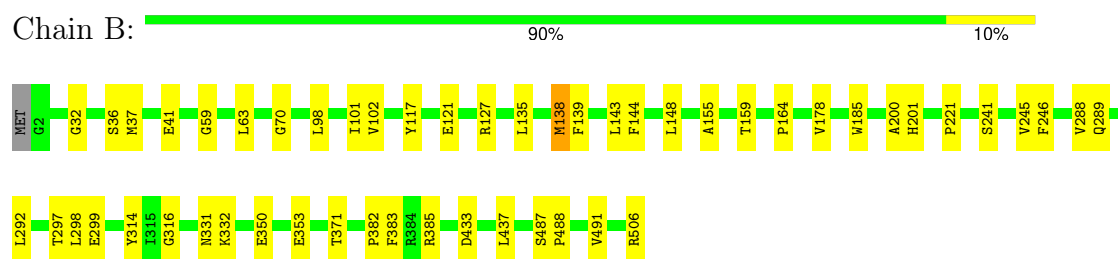
- Molecule 1: Photosystem II protein D1 1



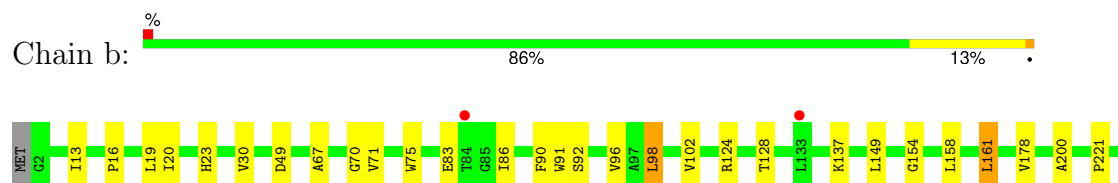
- Molecule 1: Photosystem II protein D1 1

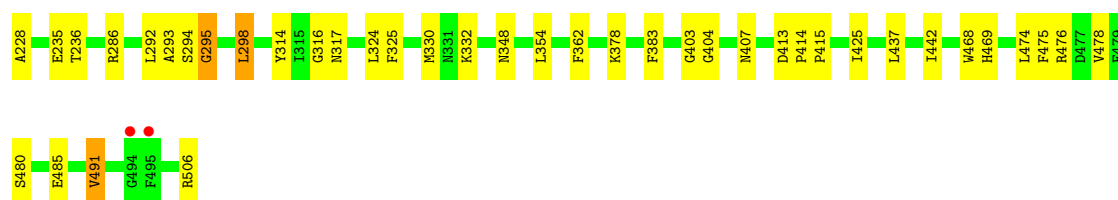


- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein





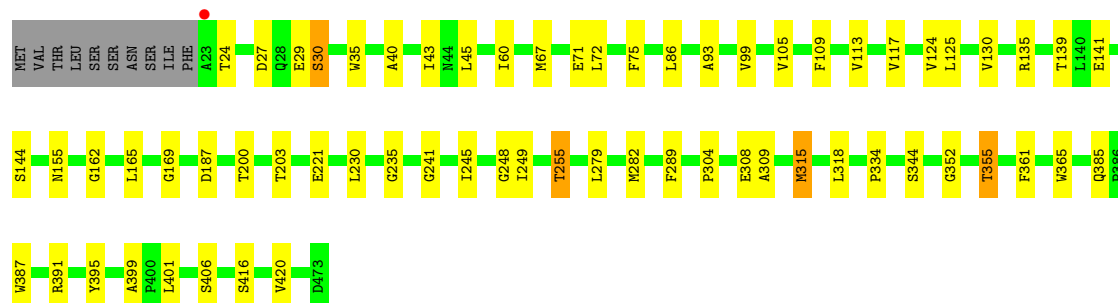
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 83% 12% ..



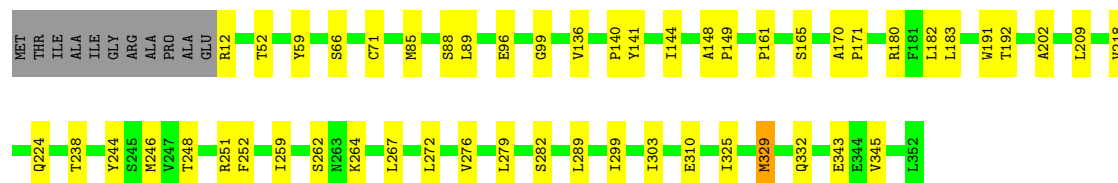
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 84% 13% ..



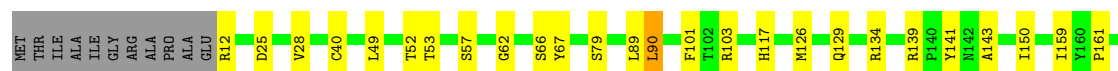
• Molecule 4: Photosystem II D2 protein

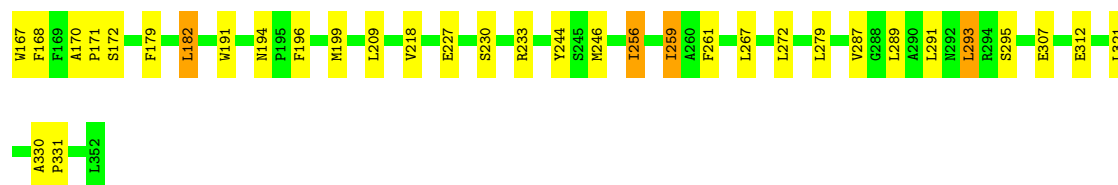
Chain D: 82% 14% .



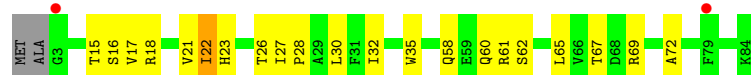
• Molecule 4: Photosystem II D2 protein

Chain d: 80% 16% ..





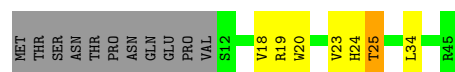
- Molecule 5: Cytochrome b559 subunit alpha



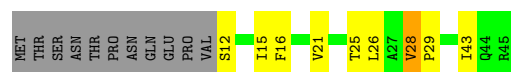
- Molecule 5: Cytochrome b559 subunit alpha



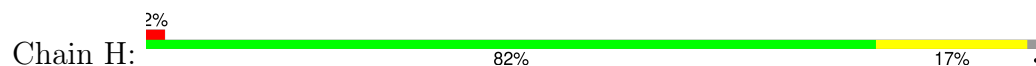
- Molecule 6: Cytochrome b559 subunit beta



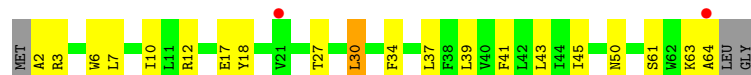
- Molecule 6: Cytochrome b559 subunit beta



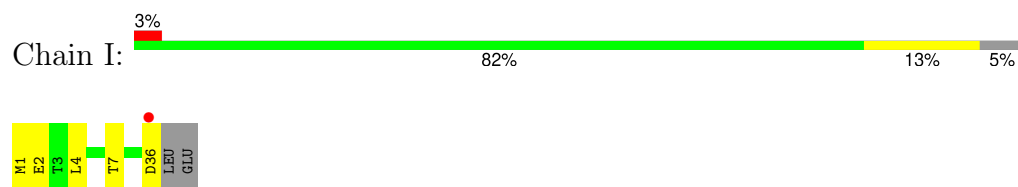
- Molecule 7: Photosystem II reaction center protein H



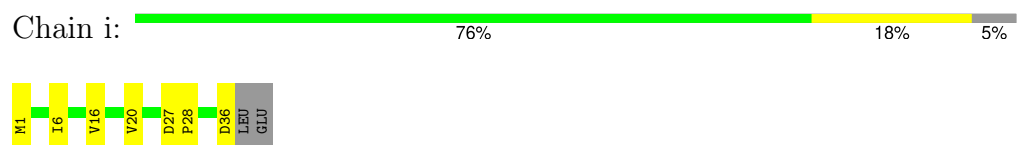
- Molecule 7: Photosystem II reaction center protein H



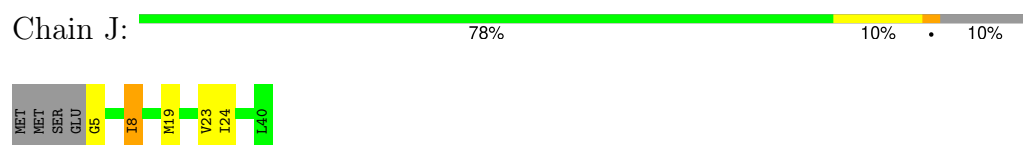
- Molecule 8: Photosystem II reaction center protein I



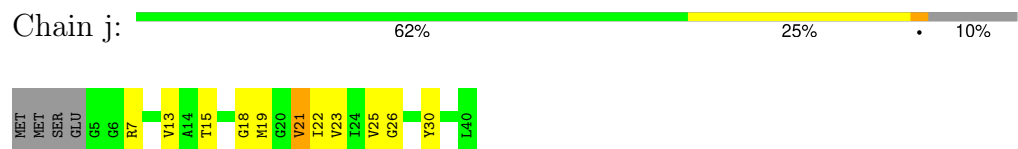
- Molecule 8: Photosystem II reaction center protein I



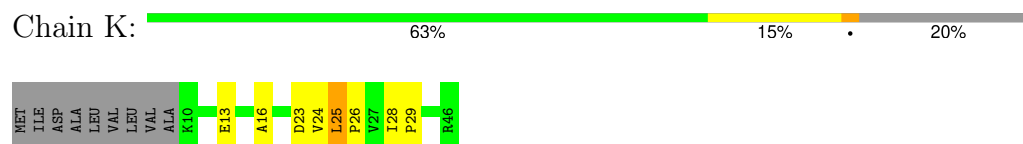
- Molecule 9: Photosystem II reaction center protein J



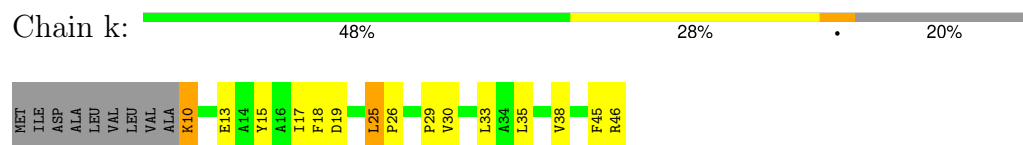
- Molecule 9: Photosystem II reaction center protein J



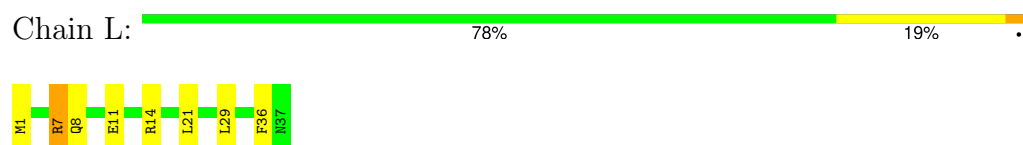
- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K

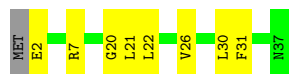


- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L

Chain l:  76% 22% .



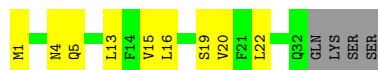
- Molecule 12: Photosystem II reaction center protein M

Chain M:  75% 14% . 8%



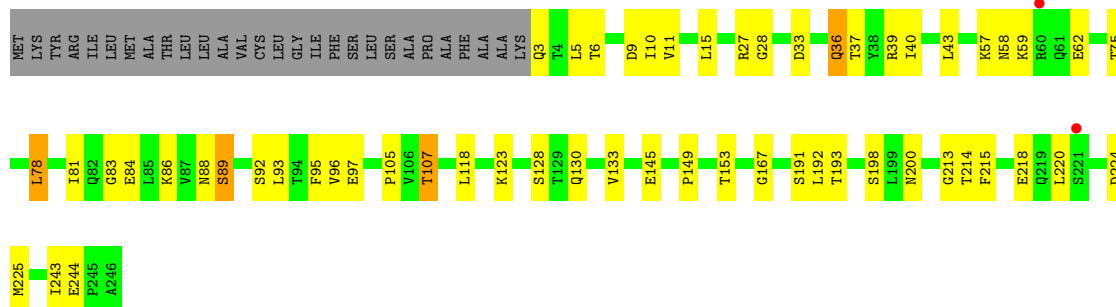
- Molecule 12: Photosystem II reaction center protein M

Chain m:  64% 25% 11%



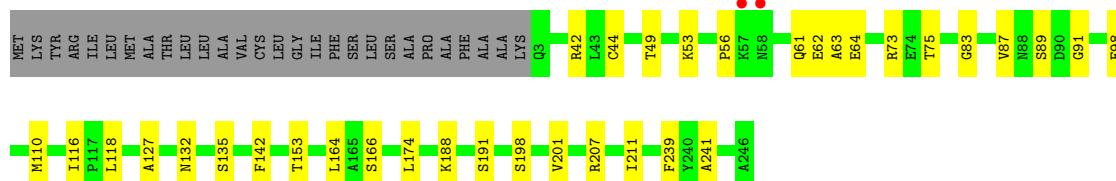
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  69% 19% . 10%



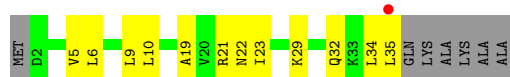
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  77% 13% 10%

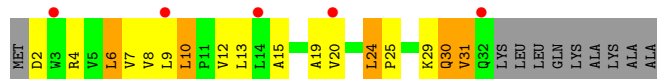


- Molecule 14: Photosystem II protein Y

Chain R:  54% 29% 17%



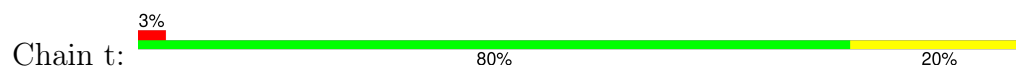
- Molecule 14: Photosystem II protein Y



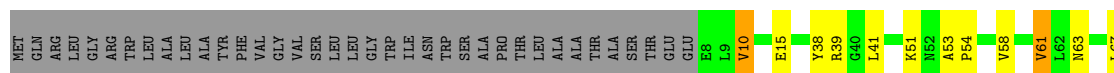
- Molecule 15: Photosystem II reaction center protein T



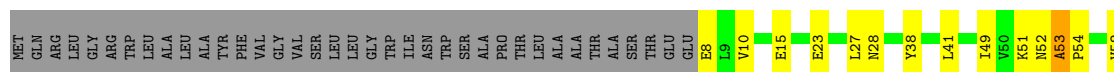
- Molecule 15: Photosystem II reaction center protein T



- Molecule 16: Photosystem II 12 kDa extrinsic protein

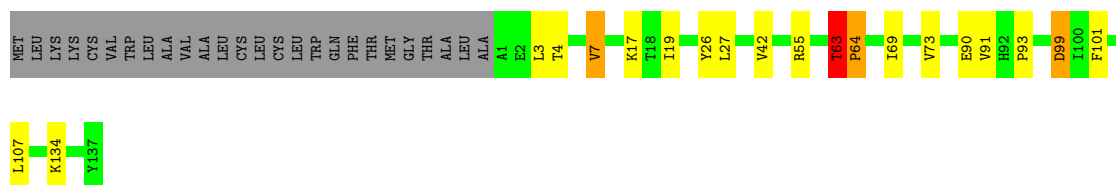


- Molecule 16: Photosystem II 12 kDa extrinsic protein

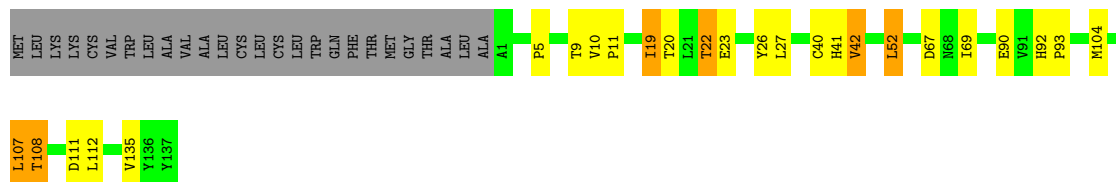


- Molecule 17: Cytochrome c-550

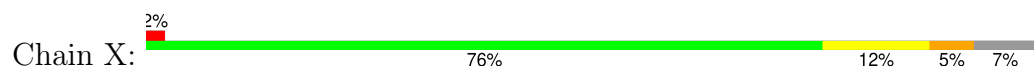




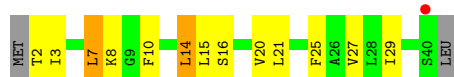
- Molecule 17: Cytochrome c-550



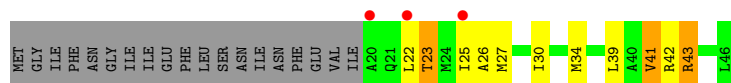
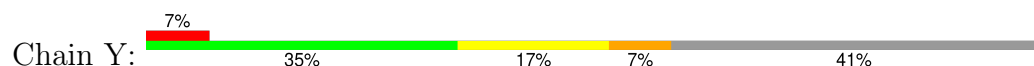
- Molecule 18: Photosystem II reaction center X protein



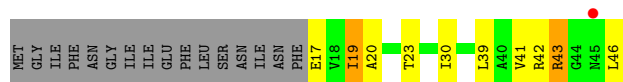
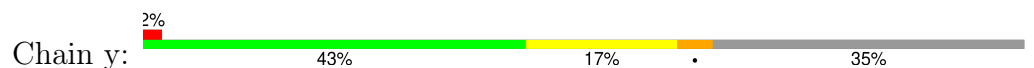
- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 19: Photosystem II reaction center protein Ycf12

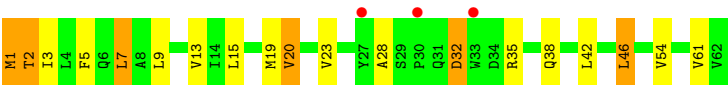


- Molecule 20: Photosystem II reaction center protein Z





● Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.07Å 222.05Å 308.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.45 – 2.27 33.45 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.5 (33.45-2.27) 84.2 (33.45-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.58 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.178 , 0.249 0.179 , 0.249	Depositor DCC
R_{free} test set	3275 reflections (0.52%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	103197	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCT, CL, STE, FE2, OEX, FME, NA, PHO, LMG, LHG, SQD, BCR, DGD, CLA, PL9, HEC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.68	0/2707	0.78	1/3692 (0.0%)
1	a	0.66	0/2704	0.76	1/3688 (0.0%)
2	B	0.64	0/4161	0.73	0/5669
2	b	0.61	0/4118	0.71	0/5611
3	C	0.62	0/3547	0.71	0/4830
3	c	0.59	0/3619	0.71	0/4926
4	D	0.68	0/2812	0.74	0/3832
4	d	0.65	0/2821	0.73	0/3844
5	E	0.56	0/688	0.65	0/940
5	e	0.52	0/683	0.62	0/932
6	F	0.52	0/284	0.65	0/387
6	f	0.51	0/284	0.67	0/387
7	H	0.67	0/523	0.73	0/713
7	h	0.53	0/511	0.67	0/697
8	I	0.62	0/293	0.76	0/396
8	i	0.62	0/293	0.69	0/396
9	J	0.54	0/263	0.72	0/356
9	j	0.51	0/263	0.71	0/356
10	K	0.51	0/303	0.64	0/416
10	k	0.46	0/303	0.61	0/416
11	L	0.68	0/311	0.71	0/422
11	l	0.69	0/303	0.68	0/412
12	M	0.66	0/249	0.69	0/341
12	m	0.69	0/244	0.79	0/334
13	O	0.62	0/1904	0.71	0/2585
13	o	0.66	0/1905	0.73	0/2583
14	R	0.48	0/277	0.64	0/380
14	r	0.37	0/246	0.51	0/339
15	T	0.70	0/257	0.81	0/349
15	t	0.67	0/255	0.68	0/346
16	U	0.58	0/785	0.69	0/1064
16	u	0.63	0/785	0.78	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.61	0/1085	0.74	1/1473 (0.1%)
17	v	0.56	0/1085	0.69	0/1473
18	X	0.55	0/284	0.66	0/384
18	x	0.49	0/289	0.64	0/391
19	Y	0.48	0/197	0.65	0/264
19	y	0.39	0/219	0.59	0/294
20	Z	0.43	0/490	0.60	0/669
20	z	0.40	0/488	0.54	0/666
All	All	0.62	0/42838	0.72	3/58317 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
16	u	0	1
17	V	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	MET	CA-CB-CG	5.13	124.36	114.10
1	a	131	TRP	CA-CB-CG	-5.05	104.00	113.60
17	V	63	THR	C-N-CD	-5.01	104.45	125.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide
16	u	52	ASN	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2622	2508	2519	20	0
1	a	2619	2499	2510	34	0
2	B	4005	3859	3867	30	0
2	b	3978	3822	3836	39	0
3	C	3426	3341	3343	37	0
3	c	3500	3413	3426	36	0
4	D	2717	2613	2621	39	0
4	d	2723	2619	2627	38	0
5	E	666	650	651	16	0
5	e	664	647	648	21	0
6	F	275	281	282	7	0
6	f	275	281	282	7	0
7	H	510	532	532	7	0
7	h	498	518	518	10	0
8	I	296	311	311	1	0
8	i	296	311	311	2	0
9	J	257	268	268	3	0
9	j	257	268	268	6	0
10	K	293	305	305	5	0
10	k	293	305	305	9	0
11	L	304	316	316	9	0
11	l	296	304	304	4	0
12	M	256	269	269	3	0
12	m	251	267	267	5	0
13	O	1870	1828	1830	35	0
13	o	1874	1844	1846	13	0
14	R	271	298	298	8	0
14	r	240	253	250	10	0
15	T	258	261	261	0	0
15	t	256	256	256	3	0
16	U	774	772	773	4	0
16	u	774	772	773	9	0
17	V	1064	1068	1073	11	0
17	v	1064	1068	1073	19	0
18	X	281	312	312	5	0
18	x	286	316	314	7	0
19	Y	196	217	217	9	0
19	y	218	241	241	8	0
20	Z	479	516	516	13	0
20	z	477	509	509	15	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	A	184	192	192	6	0
22	B	970	1067	1067	20	0
22	C	839	922	922	15	0
22	D	195	216	216	6	0
22	H	65	72	72	1	0
22	a	195	216	216	3	0
22	b	1035	1139	1139	22	0
22	c	839	919	919	14	0
22	d	195	216	216	2	0
23	A	64	74	74	0	0
23	D	64	74	74	3	0
23	a	64	74	74	1	0
23	d	64	74	74	1	0
24	A	2	0	0	0	0
24	a	2	0	0	0	0
25	A	55	80	80	4	0
25	D	55	80	80	2	0
25	a	55	80	80	1	0
25	d	55	80	80	1	0
26	A	48	66	66	0	0
26	B	28	40	40	0	0
26	D	84	114	117	1	0
26	M	51	69	72	1	0
26	Y	48	66	66	0	0
26	a	55	85	86	0	0
26	b	55	86	86	0	0
26	c	134	178	180	0	0
26	d	44	57	58	0	0
26	m	51	71	72	1	0
27	A	91	134	135	4	0
27	B	54	77	78	0	0
27	D	36	45	45	0	0
27	L	49	65	65	3	0
27	a	54	77	78	0	0
27	f	41	48	48	1	0
27	t	36	56	56	0	0
28	A	49	72	74	0	0
28	D	145	211	215	4	0
28	L	49	73	74	0	0
28	a	42	55	57	0	0
28	b	49	73	74	5	0
28	d	88	121	125	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	l	49	74	74	1	0
29	A	66	94	96	1	0
29	C	186	241	245	2	0
29	H	62	77	81	0	0
29	c	186	234	243	0	0
29	h	62	79	82	0	0
30	B	120	168	168	8	0
30	C	80	112	112	6	0
30	D	40	56	56	3	0
30	H	40	56	56	0	0
30	I	40	56	56	0	0
30	K	80	112	112	1	0
30	T	40	56	56	4	0
30	a	40	56	56	2	0
30	b	120	168	168	3	0
30	c	40	56	56	1	0
30	d	40	56	56	5	0
30	k	120	168	168	2	0
30	t	40	56	56	2	0
30	x	40	56	56	3	0
31	B	75	117	117	1	0
31	C	40	63	63	1	0
31	H	18	35	35	0	0
31	I	15	26	26	1	0
31	J	12	16	16	1	0
31	L	12	16	16	0	0
31	M	43	73	73	0	0
31	R	12	16	16	0	0
31	X	20	35	35	4	0
31	Z	8	12	12	0	0
31	a	27	42	42	0	0
31	b	131	232	232	4	0
31	c	20	35	35	1	0
31	d	17	26	26	0	0
31	j	12	16	16	1	0
31	k	12	16	16	0	0
31	t	24	36	36	1	0
31	x	20	35	35	0	0
32	C	10	0	0	0	0
32	a	10	0	0	0	0
33	D	4	1	1	0	0
33	d	4	1	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	F	43	32	32	5	0
34	V	43	30	31	1	0
34	f	43	32	32	5	0
34	v	43	30	30	4	0
35	V	1	0	0	0	0
36	A	112	0	0	2	0
36	B	142	0	0	1	0
36	C	125	0	0	1	0
36	D	96	0	0	2	0
36	E	22	0	0	0	0
36	F	6	0	0	0	0
36	H	16	0	0	1	0
36	I	10	0	0	0	0
36	J	14	0	0	1	0
36	K	3	0	0	1	0
36	L	10	0	0	4	0
36	M	9	0	0	1	0
36	O	60	0	0	5	0
36	R	11	0	0	2	0
36	T	8	0	0	0	0
36	U	28	0	0	0	0
36	V	49	0	0	2	0
36	X	10	0	0	2	0
36	Y	2	0	0	0	0
36	Z	7	0	0	0	0
36	a	96	0	0	1	0
36	b	116	0	0	1	0
36	c	108	0	0	3	0
36	d	87	0	0	0	0
36	e	11	0	0	0	0
36	f	7	0	0	1	0
36	h	17	0	0	1	0
36	i	14	0	0	0	0
36	j	8	0	0	0	0
36	k	7	0	0	1	0
36	l	11	0	0	0	0
36	m	4	0	0	1	0
36	o	67	0	0	0	0
36	r	3	0	0	1	0
36	t	8	0	0	1	0
36	u	34	0	0	2	0
36	v	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	x	6	0	0	0	0
36	y	12	0	0	2	0
36	z	6	0	0	0	0
All	All	51641	51556	51697	606	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (606) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:v:40:CYS:SG	34:v:201:HEC:CAC	2.03	1.44
18:x:3:ILE:HG23	18:x:7:LEU:HD23	1.56	0.88
1:a:229:GLU:OE1	36:a:501:HOH:O	1.97	0.82
9:J:5:GLY:N	36:J:201:HOH:O	2.12	0.82
31:X:101:STE:O1	36:X:201:HOH:O	1.99	0.81
14:r:2:ASP:N	36:r:101:HOH:O	2.12	0.81
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.18	0.79
20:z:32:ASP:N	20:z:32:ASP:OD1	2.17	0.78
3:c:40:ALA:O	3:c:43:ILE:HD12	1.84	0.78
28:b:623:LHG:O4	4:d:141:TYR:OH	2.01	0.77
17:v:104:MET:HA	17:v:107:LEU:HD22	1.67	0.77
9:j:15:THR:HG22	9:j:19:MET:HE2	1.68	0.76
4:d:267:LEU:C	4:d:267:LEU:HD23	2.10	0.76
13:O:84:GLU:OE1	13:O:86:LYS:NZ	2.18	0.76
2:B:506:ARG:O	36:B:701:HOH:O	2.05	0.75
14:R:32:GLN:NE2	36:R:201:HOH:O	2.20	0.74
22:C:513:CLA:H201	31:C:520:STE:H171	1.70	0.73
17:v:40:CYS:SG	34:v:201:HEC:C3C	2.75	0.73
20:z:15:LEU:HD22	20:z:46:LEU:HD12	1.72	0.71
7:H:3:ARG:NH1	36:H:201:HOH:O	2.23	0.71
3:C:148:GLY:O	3:C:156:LYS:NZ	2.24	0.70
22:C:508:CLA:H203	29:C:517:DGD:HAE1	1.74	0.70
30:T:101:BCR:H321	30:T:101:BCR:HC8	1.73	0.69
10:K:23:ASP:OD2	36:K:201:HOH:O	2.09	0.69
20:Z:31:GLN:O	20:Z:33:TRP:N	2.25	0.69
2:b:90:PHE:H	31:b:621:STE:H183	1.57	0.69
14:R:32:GLN:NE2	36:R:202:HOH:O	2.26	0.68
9:J:19:MET:O	9:J:23:VAL:HG23	1.93	0.68
20:z:3:ILE:HG22	20:z:7:LEU:HD22	1.76	0.68
2:B:59:GLY:O	22:B:606:CLA:HED2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:5:LEU:HD12	13:O:10:ILE:HD11	1.76	0.67
34:F:101:HEC:HBC3	34:F:101:HEC:HHD	1.74	0.67
34:v:201:HEC:HMC1	34:v:201:HEC:HBC3	1.75	0.67
20:Z:35:ARG:NH1	20:Z:38:GLN:OE1	2.28	0.67
30:t:101:BCR:H321	30:t:101:BCR:HC8	1.76	0.66
31:t:103:STE:O2	36:t:201:HOH:O	2.12	0.66
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.59	0.66
4:d:49:LEU:HD13	30:d:406:BCR:C15	2.26	0.66
7:h:3:ARG:NH2	36:h:201:HOH:O	2.28	0.66
9:j:18:GLY:O	9:j:22:ILE:HD13	1.96	0.66
19:y:17:GLU:N	36:y:101:HOH:O	2.28	0.66
16:U:58:VAL:O	16:U:61:VAL:HG22	1.96	0.65
30:d:406:BCR:H331	30:d:406:BCR:C8	2.27	0.64
5:E:22[A]:ILE:HD12	14:R:19:ALA:HB1	1.78	0.64
13:o:62:GLU:OE1	13:o:63:ALA:N	2.31	0.64
27:L:101:SQD:H121	22:b:614:CLA:H43	1.80	0.63
16:u:53:ALA:HB1	16:u:54:PRO:HD3	1.79	0.63
23:D:401:PHO:HBA2	22:D:403:CLA:H142	1.81	0.63
4:d:126:MET:HE3	4:d:143:ALA:O	1.99	0.63
17:v:40:CYS:SG	34:v:201:HEC:CBC	2.83	0.63
1:A:261:GLN:NE2	36:A:502:HOH:O	2.30	0.63
3:C:32:GLY:N	36:C:603:HOH:O	2.30	0.63
13:O:107:THR:HG22	36:O:308:HOH:O	1.98	0.63
13:O:28:GLY:O	36:O:301:HOH:O	2.16	0.63
3:C:406:SER:HA	3:C:420:VAL:HG23	1.80	0.62
22:C:512:CLA:H91	22:C:513:CLA:H141	1.80	0.62
4:D:218:VAL:HG13	4:D:244:TYR:CD1	2.34	0.62
22:B:603:CLA:H12	22:B:604:CLA:H42	1.81	0.62
22:c:511:CLA:H172	20:z:20:VAL:HG22	1.82	0.62
10:k:18:PHE:CE2	20:z:13:VAL:HG21	2.35	0.62
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.35	0.61
22:b:601:CLA:H93	30:x:101:BCR:H402	1.83	0.61
19:y:39:LEU:HB3	19:y:46:LEU:HD21	1.80	0.61
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.82	0.61
16:u:53:ALA:CB	16:u:54:PRO:CD	2.78	0.61
30:B:617:BCR:H331	30:B:617:BCR:C8	2.30	0.61
30:T:101:BCR:H382	30:T:101:BCR:H23C	1.81	0.61
16:u:53:ALA:HB1	16:u:54:PRO:CD	2.31	0.60
18:X:39:ARG:O	36:X:202:HOH:O	2.16	0.60
5:e:22:ILE:HG23	14:r:19:ALA:HB2	1.83	0.60
1:a:210:LEU:C	1:a:210:LEU:HD23	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:12:SER:N	36:f:201:HOH:O	2.35	0.60
4:d:259:ILE:HD13	4:d:259:ILE:H	1.66	0.60
3:C:334:PRO:HA	13:O:153:THR:OG1	2.02	0.60
22:C:504:CLA:H143	22:C:508:CLA:H141	1.83	0.59
22:B:605:CLA:H72	30:B:618:BCR:H311	1.83	0.59
5:E:65:LEU:O	5:E:67:THR:HG23	2.02	0.59
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.84	0.59
17:v:10:VAL:HG23	17:v:69:ILE:HD11	1.85	0.59
34:f:101:HEC:HHC	34:f:101:HEC:HBB2	1.85	0.58
19:y:17:GLU:O	19:y:20:ALA:HB3	2.03	0.58
27:L:101:SQD:O9	36:L:201:HOH:O	2.16	0.58
28:d:408:LHG:H321	15:t:21:ILE:HD11	1.85	0.58
9:j:19:MET:O	9:j:23:VAL:HG23	2.04	0.58
4:d:179:PHE:HA	4:d:182:LEU:HD22	1.84	0.58
30:D:406:BCR:H392	30:D:406:BCR:H23C	1.86	0.58
30:b:619:BCR:H331	30:b:619:BCR:C8	2.33	0.58
3:c:203:THR:O	3:c:235:GLY:HA3	2.04	0.57
4:d:279:LEU:HD22	23:d:401:PHO:HBC3	1.86	0.57
27:f:102:SQD:H331	18:x:27:VAL:HG21	1.86	0.57
30:d:406:BCR:H352	6:f:29:PRO:HB2	1.85	0.57
3:c:344:SER:O	13:o:75:THR:HG22	2.05	0.57
30:C:514:BCR:H321	30:C:514:BCR:HC8	1.87	0.57
2:B:221:PRO:HA	22:B:608:CLA:HED3	1.86	0.57
3:C:459:ILE:HG21	3:C:464:GLU:HG3	1.85	0.57
34:F:101:HEC:HHH	34:F:101:HEC:CBC	2.34	0.57
3:C:50:LEU:HD21	22:C:513:CLA:C1B	2.35	0.56
5:E:22[A]:ILE:HD11	34:F:101:HEC:CHB	2.35	0.56
13:o:110:MET:HE2	13:o:116:ILE:HD11	1.87	0.56
3:c:162:GLY:HA2	3:c:248:GLY:HA2	1.88	0.56
3:c:391[A]:ARG:NH1	36:c:603:HOH:O	2.29	0.56
29:C:517:DGD:O2D	31:J:101:STE:H21	2.06	0.56
17:v:92:HIS:ND1	17:v:93:PRO:HD2	2.21	0.56
4:D:272:LEU:C	4:D:272:LEU:HD23	2.31	0.56
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.06	0.56
4:d:126:MET:HA	4:d:129:GLN:OE1	2.05	0.56
17:V:99:ASP:N	17:V:99:ASP:OD1	2.39	0.55
34:V:201:HEC:HBC3	34:V:201:HEC:HMC3	1.87	0.55
19:Y:26:ALA:O	19:Y:30:ILE:HG22	2.06	0.55
5:e:57:ALA:HB3	5:e:60:GLN:HG2	1.89	0.55
19:Y:23:THR:HG22	19:Y:27:MET:HE3	1.88	0.55
3:c:27:ASP:OD1	3:c:30:SER:OG	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:z:3:ILE:HG22	20:z:7:LEU:CD2	2.36	0.55
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.71	0.55
1:a:114:LEU:C	1:a:114:LEU:HD23	2.32	0.55
17:v:26:TYR:HD2	17:v:27:LEU:HD23	1.71	0.55
34:F:101:HEC:HBB2	34:F:101:HEC:HMB3	1.89	0.55
19:Y:41:VAL:HG12	19:Y:42:ARG:N	2.22	0.55
25:A:408:PL9:C36	6:F:25:THR:HG21	2.36	0.55
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.89	0.55
22:b:613:CLA:H192	28:b:623:LHG:H221	1.88	0.55
16:u:58:VAL:HG12	16:u:79:LEU:HD22	1.89	0.55
10:K:24:VAL:HG21	19:Y:25:ILE:HB	1.88	0.54
5:e:68:ASP:O	5:e:72:ALA:HB2	2.07	0.54
16:U:38:TYR:HB2	16:U:41:LEU:HD12	1.88	0.54
1:a:263:ALA:O	25:a:409:PL9:H152	2.07	0.54
30:C:514:BCR:H321	30:C:514:BCR:C8	2.38	0.54
4:D:267:LEU:C	4:D:267:LEU:HD23	2.31	0.54
10:k:18:PHE:HE2	20:z:13:VAL:HG21	1.73	0.54
13:O:10:ILE:HG23	13:O:15:LEU:HB2	1.88	0.54
5:E:23:HIS:HB3	5:E:27:ILE:HD12	1.90	0.54
19:Y:39:LEU:HD21	20:Z:28:ALA:HB3	1.89	0.54
1:a:95:PRO:HD2	1:a:98:GLU:HG3	1.90	0.53
3:C:61:VAL:HG12	3:C:118:HIS:O	2.09	0.53
22:a:402:CLA:HBB1	22:a:402:CLA:HMB3	1.90	0.53
4:d:40:CYS:HB3	4:d:117:HIS:O	2.09	0.53
4:D:99:GLY:HA3	31:X:101:STE:H21	1.89	0.53
4:D:218:VAL:HG22	4:D:244:TYR:CZ	2.43	0.53
3:C:141:GLU:H	3:C:141:GLU:CD	2.17	0.53
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.24	0.53
1:a:291:SER:O	1:a:294:ALA:HB3	2.08	0.53
4:d:89:LEU:HD12	7:h:50:ASN:OD1	2.08	0.53
4:D:279:LEU:HD22	23:D:401:PHO:HBC3	1.91	0.53
12:m:4:ASN:ND2	26:m:101:LMG:O10	2.42	0.53
2:b:92:SER:O	2:b:96:VAL:HG23	2.10	0.52
22:c:501:CLA:H192	22:c:507:CLA:HBB1	1.91	0.52
17:V:63:THR:HG22	17:V:64:PRO:CD	2.39	0.52
4:d:62:GLY:HA2	5:e:63:ILE:HG21	1.92	0.52
36:u:201:HOH:O	17:v:135:VAL:HG23	2.08	0.52
3:C:109:PHE:N	3:C:110:PRO:CD	2.72	0.52
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.90	0.52
22:c:510:CLA:H201	10:k:33:LEU:HD22	1.92	0.52
4:D:218:VAL:HG22	4:D:244:TYR:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:45:GLY:HA2	20:Z:48:ILE:HD12	1.91	0.52
22:b:607:CLA:H91	11:l:31:PHE:CE1	2.44	0.52
1:a:84:PRO:HA	1:a:112:TYR:CG	2.44	0.52
23:a:404:PHO:HBB1	23:a:404:PHO:HMB3	1.92	0.52
1:A:332:HIS:O	1:A:333:GLU:C	2.52	0.52
3:C:203:THR:O	3:C:235:GLY:HA3	2.09	0.52
3:C:216:SER:HB3	3:C:221:GLU:HG3	1.92	0.52
2:b:16:PRO:O	2:b:20:ILE:HD12	2.08	0.52
1:a:229:GLU:CD	1:a:229:GLU:H	2.18	0.51
1:a:306:VAL:HG12	1:a:314:ILE:HB	1.93	0.51
6:f:21:VAL:O	6:f:25:THR:HG23	2.10	0.51
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.46	0.51
20:z:9:LEU:HD13	20:z:54:VAL:HG11	1.92	0.51
2:B:135:LEU:HA	2:B:138:MET:HG3	1.92	0.51
22:B:607:CLA:H191	4:D:89:LEU:HD13	1.92	0.51
4:D:59:TYR:O	5:E:65:LEU:HD12	2.11	0.51
2:B:102:VAL:HA	30:B:617:BCR:C40	2.40	0.51
4:d:209:LEU:HD23	4:d:209:LEU:C	2.35	0.51
2:B:241:SER:O	2:B:245:VAL:HG23	2.09	0.51
3:c:130:VAL:HG21	22:c:511:CLA:H151	1.92	0.51
4:d:246:MET:HE2	4:d:246:MET:HA	1.93	0.51
7:h:63:LYS:O	7:h:64:ALA:HB2	2.11	0.51
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.92	0.51
10:K:28:ILE:N	10:K:29:PRO:CD	2.74	0.51
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.93	0.51
16:u:8:GLU:N	36:u:204:HOH:O	2.43	0.51
2:B:144:PHE:CE2	2:B:148:LEU:HD11	2.45	0.50
4:D:141:TYR:OH	28:D:413:LHG:O4	2.18	0.50
16:U:10:VAL:HG21	16:U:15:GLU:OE2	2.11	0.50
31:I:102:STE:H131	22:b:606:CLA:H192	1.92	0.50
13:O:5:LEU:CD1	13:O:10:ILE:HD11	2.40	0.50
1:a:257:ARG:NH1	2:b:491:VAL:O	2.40	0.50
7:h:30:LEU:HD12	7:h:34:PHE:CE2	2.46	0.50
13:O:27:ARG:NH1	36:O:304:HOH:O	2.34	0.50
3:C:95:LEU:HD21	22:C:501:CLA:OBD	2.11	0.50
13:O:27:ARG:O	13:O:27:ARG:HG2	2.12	0.50
22:b:605:CLA:HHC	22:b:605:CLA:HBB1	1.94	0.50
22:b:605:CLA:H142	22:b:610:CLA:C2	2.42	0.50
5:e:13:ILE:HG22	5:e:19:TYR:CD2	2.47	0.50
22:B:613:CLA:H141	22:B:613:CLA:H171	1.93	0.50
2:B:185:TRP:HB3	22:H:101:CLA:HMA3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:61:VAL:O	20:Z:62:VAL:C	2.55	0.50
2:b:314:TYR:CE2	2:b:316:GLY:HA3	2.47	0.50
1:a:210:LEU:HD23	1:a:210:LEU:O	2.11	0.50
5:e:30:LEU:HD11	34:f:101:HEC:CBB	2.42	0.50
4:D:332:GLN:NE2	36:D:504:HOH:O	2.39	0.49
11:L:7:ARG:NH2	36:L:203:HOH:O	2.45	0.49
20:Z:51:VAL:O	20:Z:54:VAL:O	2.29	0.49
5:e:32:ILE:O	5:e:36:LEU:HG	2.12	0.49
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.47	0.49
1:a:278:TRP:HB3	1:a:279:PRO:HD3	1.95	0.49
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.94	0.49
3:c:406:SER:HA	3:c:420:VAL:HG23	1.93	0.49
5:e:26:THR:HA	14:r:15:ALA:HB1	1.94	0.49
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.48	0.49
22:B:608:CLA:H203	7:H:39:LEU:CD1	2.42	0.49
5:E:18:ARG:HE	14:R:23:ILE:HD12	1.77	0.49
22:c:509:CLA:H43	22:c:509:CLA:O1A	2.13	0.49
3:c:187:ASP:HB2	3:c:230:LEU:HD12	1.94	0.49
10:K:25:LEU:N	10:K:26:PRO:HD2	2.27	0.49
28:b:623:LHG:HC91	28:l:101:LHG:HC81	1.94	0.49
10:k:19:ASP:OD1	36:k:201:HOH:O	2.20	0.49
18:x:3:ILE:HG23	18:x:7:LEU:CD2	2.36	0.49
19:y:39:LEU:HD21	20:z:28:ALA:HB3	1.94	0.49
4:D:282:SER:HB2	22:D:403:CLA:O1D	2.12	0.49
5:E:17:VAL:O	5:E:21:VAL:HG23	2.13	0.49
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.48	0.49
1:a:289:GLY:O	1:a:293:MET:HE3	2.13	0.49
3:c:71:GLU:HB3	3:c:86:LEU:HD22	1.94	0.49
22:d:404:CLA:H43	22:d:404:CLA:O1A	2.12	0.49
4:D:246:MET:HE2	4:D:246:MET:HA	1.94	0.49
1:A:114:LEU:C	1:A:114:LEU:HD23	2.39	0.48
14:R:34:LEU:O	14:R:35:LEU:O	2.31	0.48
3:C:443:TRP:CZ2	22:C:508:CLA:HMD1	2.49	0.48
22:b:613:CLA:H192	28:b:623:LHG:C22	2.43	0.48
3:c:391[B]:ARG:CZ	36:c:603:HOH:O	2.60	0.48
14:r:20:VAL:O	14:r:24:LEU:HB2	2.14	0.48
20:z:1:MET:O	20:z:2:THR:C	2.57	0.48
18:x:3:ILE:CG2	18:x:7:LEU:HD23	2.35	0.48
19:y:42:ARG:O	19:y:43:ARG:C	2.56	0.48
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.48	0.48
4:D:246:MET:HE3	4:D:264:LYS:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:v:5:PRO:O	17:v:9:THR:OG1	2.29	0.48
20:z:19:MET:O	20:z:23:VAL:HG23	2.13	0.48
1:A:97:TRP:HA	8:I:1:FME:HG2	1.95	0.48
4:D:310:GLU:HG3	13:O:224:ASP:OD2	2.12	0.48
19:Y:42:ARG:HH12	20:Z:31:GLN:NE2	2.12	0.48
3:c:309:ALA:HB1	3:c:399:ALA:HB2	1.96	0.48
25:A:408:PL9:H361	6:F:25:THR:HG21	1.95	0.48
11:L:8:GLN:NE2	36:L:202:HOH:O	2.36	0.47
3:C:50:LEU:O	3:C:54:VAL:HG23	2.14	0.47
22:b:605:CLA:H8	22:b:612:CLA:H201	1.97	0.47
34:f:101:HEC:HBC2	34:f:101:HEC:CMC	2.44	0.47
13:o:91:GLY:HA3	13:o:132:ASN:HA	1.96	0.47
17:v:67:ASP:OD1	17:v:67:ASP:N	2.43	0.47
25:A:408:PL9:H362	6:F:25:THR:HG21	1.95	0.47
3:C:213:LEU:HD21	30:C:514:BCR:C20	2.44	0.47
26:M:101:LMG:HC71	26:M:101:LMG:O9	2.13	0.47
2:b:324:LEU:HD23	2:b:325:PHE:CE2	2.49	0.47
10:K:26:PRO:O	10:K:29:PRO:HD2	2.14	0.47
12:M:5:GLN:NE2	36:M:202:HOH:O	2.48	0.47
2:b:292:LEU:HD21	2:b:298:LEU:HD23	1.96	0.47
2:B:288:VAL:O	2:B:292:LEU:HG	2.14	0.47
3:C:337:LEU:HD23	13:O:105:PRO:HG2	1.96	0.47
28:D:411:LHG:H141	28:D:411:LHG:H322	1.95	0.47
14:R:5:VAL:O	14:R:9:LEU:HG	2.13	0.47
5:e:25:ILE:HD12	5:e:25:ILE:N	2.30	0.47
22:B:603:CLA:H93	22:B:604:CLA:HAB	1.97	0.47
1:a:77:ILE:HD11	15:t:6:TYR:HB3	1.96	0.47
22:d:404:CLA:H52	25:d:407:PL9:H151	1.95	0.47
13:o:83:GLY:HA2	13:o:98:GLU:HG3	1.97	0.47
3:C:348:GLU:OE2	13:O:11:VAL:HA	2.14	0.47
17:V:90:GLU:HB2	17:V:91:VAL:HG13	1.96	0.46
10:k:15:TYR:CZ	20:z:5:PHE:HZ	2.34	0.46
1:A:183:MET:HA	22:A:402:CLA:HMD1	1.96	0.46
22:B:613:CLA:H203	31:B:623:STE:H121	1.97	0.46
3:c:282:MET:HE1	22:c:507:CLA:H11	1.97	0.46
30:c:514:BCR:C8	30:c:514:BCR:H331	2.44	0.46
17:v:10:VAL:CG2	17:v:69:ILE:HD11	2.45	0.46
3:c:141:GLU:HB2	36:c:639:HOH:O	2.14	0.46
16:u:38:TYR:HB2	16:u:41:LEU:HD12	1.96	0.46
4:d:259:ILE:HD13	4:d:259:ILE:N	2.28	0.46
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:402:CLA:HBB1	22:A:402:CLA:HMB3	1.97	0.46
22:B:603:CLA:H41	22:B:603:CLA:H61	1.56	0.46
22:B:609:CLA:HBD	22:B:609:CLA:H143	1.96	0.46
3:C:223:TRP:CG	3:C:224:ILE:H	2.32	0.46
4:d:170:ALA:HB1	4:d:171:PRO:CD	2.46	0.46
2:b:67:ALA:HA	2:b:71:VAL:O	2.16	0.46
2:b:474:LEU:O	4:d:134:ARG:NH1	2.49	0.46
22:A:403:CLA:HMD2	4:D:182:LEU:HD11	1.97	0.46
2:B:200:ALA:O	2:B:201:HIS:C	2.57	0.46
2:b:442:ILE:HD11	13:o:174:LEU:HD23	1.98	0.46
3:c:334:PRO:HA	13:o:153:THR:OG1	2.15	0.46
9:j:30:TYR:HA	31:j:101:STE:H22	1.98	0.46
1:A:116:ILE:HG13	1:A:117:PHE:N	2.31	0.46
3:C:241:GLY:O	3:C:245:ILE:HG13	2.15	0.46
11:L:14:ARG:HH22	27:L:101:SQD:H3	1.81	0.46
13:O:193:THR:HG21	13:O:220:LEU:HD12	1.97	0.46
13:O:215:PHE:C	13:O:215:PHE:CD1	2.94	0.46
2:b:293:ALA:C	2:b:295:GLY:H	2.23	0.46
16:u:92:VAL:HG12	16:u:97:ARG:HD2	1.96	0.46
18:x:10:PHE:CE2	18:x:14:LEU:HD22	2.50	0.46
22:A:403:CLA:H91	26:D:408:LMG:H242	1.98	0.46
22:B:613:CLA:H61	22:B:613:CLA:H41	1.72	0.46
16:U:53:ALA:HB1	16:U:54:PRO:HA	1.98	0.46
2:b:235:GLU:OE1	2:b:469:HIS:ND1	2.28	0.46
3:c:155:ASN:OD1	3:c:255:THR:HG22	2.16	0.46
8:i:16:VAL:O	8:i:20:VAL:HG23	2.16	0.46
2:b:154:GLY:HA2	2:b:158:LEU:HD12	1.97	0.46
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.51	0.46
3:c:117:VAL:HG22	30:k:101:BCR:H342	1.97	0.45
17:v:19:ILE:HD13	17:v:20:THR:N	2.31	0.45
30:x:101:BCR:C8	30:x:101:BCR:H331	2.46	0.45
1:A:85:SER:HA	1:A:109:GLY:HA3	1.99	0.45
4:D:66:SER:O	4:D:71:CYS:HB2	2.16	0.45
30:K:102:BCR:H321	30:K:102:BCR:HC8	1.98	0.45
17:V:69:ILE:O	17:V:73:VAL:HG23	2.16	0.45
19:Y:30:ILE:O	19:Y:30:ILE:HD12	2.17	0.45
1:a:131:TRP:CE3	1:a:132:GLU:HA	2.51	0.45
1:a:210:LEU:C	1:a:210:LEU:CD2	2.88	0.45
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.52	0.45
2:B:139:PHE:CZ	2:B:143:LEU:HD22	2.51	0.45
3:C:140:LEU:O	3:C:142:GLU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:60:GLN:NE2	5:E:62:SER:OG	2.50	0.45
30:b:618:BCR:C8	30:b:618:BCR:H331	2.46	0.45
4:d:57:SER:OG	4:d:79:SER:HB2	2.16	0.45
14:r:8:VAL:HG12	14:r:8:VAL:O	2.16	0.45
4:D:85:MET:HE1	5:E:72:ALA:HB2	1.98	0.45
13:O:33:ASP:O	13:O:36:GLN:N	2.46	0.45
2:b:98:LEU:HD22	2:b:102:VAL:HG23	1.99	0.45
3:c:117:VAL:HG11	31:c:519:STE:H132	1.99	0.45
5:E:22[B]:ILE:HG23	14:R:19:ALA:HB2	1.97	0.45
13:O:78:LEU:HB3	13:O:81:ILE:HD11	1.99	0.45
13:O:93:LEU:O	13:O:128:SER:HA	2.17	0.45
2:b:378:LYS:HE3	36:b:708:HOH:O	2.16	0.45
22:b:605:CLA:HMC3	22:b:615:CLA:H43	1.99	0.45
4:d:267:LEU:HD23	4:d:267:LEU:O	2.16	0.45
18:X:17:GLY:HA2	31:X:101:STE:H141	1.98	0.45
5:e:24:SER:C	5:e:25:ILE:HD12	2.42	0.45
22:B:610:CLA:HBB1	22:B:610:CLA:HMB3	1.99	0.45
3:c:60:ILE:HG22	22:c:503:CLA:HHD	1.98	0.45
4:d:267:LEU:C	4:d:267:LEU:CD2	2.85	0.45
30:d:406:BCR:H402	9:j:21:VAL:HG21	1.98	0.45
3:C:264:PHE:CZ	30:C:514:BCR:H322	2.52	0.45
7:H:25:TRP:O	7:H:26:GLY:C	2.60	0.45
19:Y:22:LEU:HA	19:Y:25:ILE:HG22	1.99	0.45
20:Z:5:PHE:CD1	20:Z:5:PHE:C	2.94	0.45
1:a:301:ASN:C	1:a:301:ASN:OD1	2.59	0.45
9:j:25:VAL:O	9:j:26:GLY:C	2.58	0.45
4:D:192:THR:HG23	22:D:403:CLA:HBC2	1.99	0.45
20:Z:31:GLN:NE2	20:Z:32:ASP:HB2	2.31	0.45
22:b:601:CLA:HBC3	22:b:601:CLA:HHD	1.99	0.45
4:d:79:SER:HA	4:d:172:SER:HB3	1.97	0.45
4:d:330:ALA:HB3	4:d:331:PRO:HD3	1.99	0.45
30:d:406:BCR:H331	30:d:406:BCR:HC8	1.97	0.45
13:O:123:LYS:NZ	36:O:305:HOH:O	2.35	0.45
2:b:468:TRP:CH2	28:b:623:LHG:HC42	2.52	0.45
2:B:155:ALA:O	2:B:159:THR:OG1	2.28	0.44
2:B:164:PRO:HG3	22:B:605:CLA:O1D	2.16	0.44
2:b:403:GLY:O	2:b:407:ASN:HB2	2.17	0.44
5:e:30:LEU:HD11	34:f:101:HEC:HBB1	2.00	0.44
13:o:44:CYS:O	13:o:239:PHE:HA	2.17	0.44
3:C:276:LEU:HD23	3:C:437:PHE:CD2	2.52	0.44
18:X:3:ILE:HG13	18:X:3:ILE:O	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:324:LEU:HD12	4:d:293:LEU:HD13	1.99	0.44
17:v:108:THR:HG23	17:v:111:ASP:OD2	2.18	0.44
4:D:12:ARG:NE	4:D:12:ARG:HA	2.32	0.44
13:O:57:LYS:HD3	2:b:49:ASP:OD2	2.18	0.44
22:b:601:CLA:HBB2	30:x:101:BCR:H351	2.00	0.44
2:b:91:TRP:HE1	31:b:621:STE:H111	1.82	0.44
5:e:5:THR:OG1	5:e:7:GLU:OE1	2.32	0.44
7:h:6:TRP:NE1	7:h:10:ILE:HD11	2.32	0.44
27:A:410:SQD:H262	28:D:411:LHG:H122	2.00	0.44
27:A:412:SQD:H383	22:b:606:CLA:H93	2.00	0.44
30:C:514:BCR:H15C	30:C:514:BCR:H351	1.80	0.44
2:b:332:LYS:NZ	2:b:437:LEU:O	2.44	0.44
3:c:385:GLN:HB2	3:c:387:TRP:CD1	2.53	0.44
4:d:194:ASN:HA	4:d:295:SER:OG	2.18	0.44
6:f:16:PHE:H	14:r:30:GLN:HE22	1.66	0.44
7:h:41:PHE:CZ	7:h:45:ILE:HD11	2.53	0.44
20:z:2:THR:O	20:z:3:ILE:C	2.61	0.44
2:B:36:SER:OG	30:B:617:BCR:H362	2.17	0.44
2:B:121:GLU:OE1	7:H:12:ARG:NH2	2.51	0.44
5:e:14:ILE:O	5:e:20:TRP:NE1	2.49	0.44
17:v:41:HIS:O	17:v:42:VAL:C	2.59	0.44
1:A:322:ASN:OD1	3:C:412:THR:HA	2.18	0.44
20:z:38:GLN:O	20:z:42:LEU:HD23	2.17	0.44
13:O:83:GLY:HA3	13:O:96:VAL:O	2.18	0.44
2:b:30:VAL:HG12	22:b:605:CLA:HHD	1.99	0.44
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.46	0.44
2:B:299[B]:GLU:H	2:B:299[B]:GLU:CD	2.26	0.43
15:t:15:ALA:O	15:t:19:PHE:HD1	2.01	0.43
13:O:93:LEU:HD11	13:O:133:VAL:HG11	1.99	0.43
1:a:153:SER:HB3	22:a:402:CLA:H43	1.99	0.43
1:A:131:TRP:CD2	1:A:131:TRP:C	2.93	0.43
1:A:192:ILE:HG13	1:A:293:MET:HE1	2.00	0.43
4:D:325:ILE:O	4:D:329:MET:HB3	2.19	0.43
13:O:149:PRO:HA	13:O:192:LEU:HD12	2.00	0.43
2:b:383:PHE:O	13:o:166:SER:HA	2.19	0.43
20:z:32:ASP:HA	20:z:35:ARG:HG3	2.00	0.43
1:A:40:THR:O	1:A:118:HIS:HB3	2.17	0.43
36:A:516:HOH:O	13:O:107:THR:HG21	2.17	0.43
12:M:20:VAL:HG11	12:m:20:VAL:HG22	2.01	0.43
13:O:145:GLU:HB3	36:O:315:HOH:O	2.18	0.43
2:b:161:LEU:HD23	2:b:161:LEU:HA	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:218:VAL:HG22	4:d:244:TYR:CZ	2.53	0.43
10:k:25:LEU:N	10:k:26:PRO:CD	2.81	0.43
30:t:101:BCR:H321	30:t:101:BCR:C8	2.47	0.43
30:a:406:BCR:C8	30:a:406:BCR:H331	2.48	0.43
5:e:40:THR:HB	14:r:4:ARG:HD2	2.01	0.43
12:m:15:VAL:O	12:m:19:SER:OG	2.30	0.43
18:x:16:SER:O	18:x:20:VAL:HG23	2.18	0.43
3:C:343:ARG:NH2	3:C:347:GLY:O	2.48	0.43
13:O:88:ASN:O	13:O:89:SER:C	2.62	0.43
18:X:29:ILE:O	18:X:33:GLN:HG2	2.17	0.43
1:a:207:GLY:O	1:a:211:PHE:CD2	2.71	0.43
2:b:414:PRO:N	2:b:415:PRO:CD	2.81	0.43
3:c:67:MET:O	3:c:71:GLU:HG3	2.19	0.43
14:r:24:LEU:N	14:r:25:PRO:HD2	2.33	0.43
17:v:22:THR:O	17:v:23:GLU:C	2.62	0.43
4:D:251:ARG:O	4:D:252:PHE:C	2.62	0.43
3:c:245:ILE:O	3:c:249:ILE:HD12	2.19	0.43
3:c:352:GLY:O	3:c:355:THR:HG22	2.18	0.43
22:c:513:CLA:HBB1	22:c:513:CLA:HMB1	2.00	0.43
4:D:299:ILE:HG22	4:D:303:ILE:HD12	2.00	0.43
22:D:403:CLA:H193	22:D:403:CLA:H162	1.89	0.43
6:F:20:TRP:CE2	6:F:24:HIS:CE1	3.06	0.43
1:a:279:PRO:O	1:a:283:VAL:HG23	2.19	0.43
3:c:35:TRP:CD1	10:k:45:PHE:HB3	2.53	0.43
2:B:332:LYS:O	2:B:332:LYS:HG3	2.17	0.43
22:B:601:CLA:C4	7:H:45:ILE:HG22	2.48	0.43
4:D:96:GLU:HB2	36:D:535:HOH:O	2.19	0.43
2:b:19:LEU:HD11	2:b:23:HIS:NE2	2.34	0.43
22:b:613:CLA:HED2	22:b:614:CLA:HMC2	2.01	0.43
22:c:501:CLA:C3D	22:c:503:CLA:H2	2.49	0.43
10:k:10:LYS:HD2	10:k:10:LYS:N	2.34	0.43
13:o:127:ALA:HB1	13:o:142:PHE:HB3	2.01	0.43
17:v:26:TYR:CD2	17:v:27:LEU:HD23	2.53	0.43
18:x:25:PHE:O	18:x:29:ILE:HG13	2.19	0.43
3:C:278:ALA:CB	22:C:501:CLA:H141	2.49	0.43
3:C:344:SER:O	13:O:75:THR:HG22	2.19	0.43
11:L:7:ARG:HG2	11:L:7:ARG:HH21	1.84	0.43
3:c:45:LEU:HA	3:c:139:THR:HG22	2.01	0.43
4:d:261:PHE:CZ	28:d:408:LHG:HC81	2.53	0.43
11:l:20:GLY:HA3	12:m:22:LEU:HD13	1.99	0.43
3:C:93:ALA:HB1	3:C:99:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.49	0.42
5:E:35:TRP:CD1	5:E:35:TRP:C	2.96	0.42
20:Z:31:GLN:NE2	20:Z:32:ASP:H	2.17	0.42
3:c:318:LEU:C	3:c:318:LEU:HD23	2.44	0.42
1:A:307:ILE:HG22	1:A:313:VAL:HA	2.00	0.42
2:B:382:PRO:HG2	2:B:385:ARG:HD2	2.00	0.42
3:C:319:ILE:HD13	3:C:389:GLU:HG3	2.01	0.42
13:O:92:SER:HA	13:O:130:GLN:O	2.20	0.42
31:b:628:STE:H72	31:b:629:STE:H81	2.00	0.42
4:d:159:ILE:HG21	4:d:287:VAL:HG22	2.01	0.42
12:m:5:GLN:O	36:m:201:HOH:O	2.22	0.42
22:B:603:CLA:C1	22:B:604:CLA:H42	2.48	0.42
22:C:507:CLA:H92	22:C:507:CLA:H61	1.86	0.42
11:L:21:LEU:HD23	11:L:21:LEU:HA	1.84	0.42
7:h:61:SER:C	7:h:63:LYS:N	2.77	0.42
19:y:19:ILE:C	19:y:19:ILE:HD13	2.44	0.42
22:B:612:CLA:H171	30:B:617:BCR:H312	2.01	0.42
3:C:112:PHE:O	3:C:116:VAL:HG23	2.19	0.42
25:D:407:PL9:H412	11:L:29:LEU:HD23	2.00	0.42
17:V:4:THR:O	17:V:7:VAL:HG13	2.20	0.42
17:V:107:LEU:HD23	17:V:107:LEU:HA	1.86	0.42
2:b:221:PRO:HB3	22:b:609:CLA:O1D	2.19	0.42
8:i:27:ASP:N	8:i:28:PRO:CD	2.81	0.42
17:v:52:LEU:HD12	17:v:52:LEU:HA	1.79	0.42
2:B:246:PHE:CD1	2:B:246:PHE:C	2.97	0.42
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.00	0.42
11:L:36:PHE:HB3	12:M:3:VAL:HB	2.02	0.42
17:V:26:TYR:CD2	17:V:27:LEU:HD23	2.55	0.42
2:b:475:PHE:O	2:b:476:ARG:C	2.63	0.42
3:c:93:ALA:HB1	3:c:99:VAL:HG21	2.01	0.42
2:B:117:TYR:HA	11:L:1:MET:HE1	2.01	0.42
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.90	0.42
6:f:26:LEU:O	6:f:29:PRO:HD2	2.18	0.42
13:o:42:ARG:O	13:o:241:ALA:HA	2.20	0.42
2:B:32:GLY:HA3	30:B:617:BCR:C17	2.50	0.42
3:C:223:TRP:CE3	3:C:224:ILE:HG12	2.54	0.42
22:C:513:CLA:HHC	22:C:513:CLA:HBB1	2.00	0.42
30:C:514:BCR:H24C	30:C:514:BCR:H371	1.90	0.42
4:D:52:THR:O	4:D:66:SER:HA	2.20	0.42
1:a:278:TRP:HB3	1:a:279:PRO:CD	2.50	0.42
2:b:200:ALA:HB1	22:b:602:CLA:HBB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:607:CLA:H172	22:B:608:CLA:H193	2.02	0.42
3:C:278:ALA:HB1	22:C:501:CLA:H141	2.02	0.42
4:D:209:LEU:HD23	4:D:209:LEU:C	2.44	0.42
30:D:406:BCR:C8	30:D:406:BCR:H331	2.49	0.42
30:D:406:BCR:H20C	30:D:406:BCR:H361	1.85	0.42
13:O:36:GLN:HG3	13:O:37:THR:N	2.35	0.42
1:a:237:TYR:HB2	1:a:245:THR:HG21	2.01	0.42
2:b:413:ASP:HA	2:b:414:PRO:HD3	1.95	0.42
22:b:607:CLA:H62	22:b:607:CLA:H41	1.86	0.42
22:c:508:CLA:HMD3	28:d:409:LHG:H102	2.02	0.42
13:o:201:VAL:HG22	13:o:211:ILE:HD12	2.01	0.42
22:A:403:CLA:HMB1	22:A:403:CLA:HBB1	2.02	0.42
22:B:601:CLA:H43	7:H:45:ILE:HG22	2.01	0.42
28:d:408:LHG:H152	11:l:22:LEU:HD21	2.01	0.42
5:e:30:LEU:HD23	5:e:30:LEU:HA	1.90	0.42
17:v:11:PRO:O	17:v:69:ILE:HD12	2.20	0.42
6:F:23:VAL:HG11	34:F:101:HEC:CMD	2.50	0.41
20:Z:52:LEU:O	20:Z:56:VAL:HG23	2.19	0.41
2:b:19:LEU:HD11	2:b:23:HIS:CE1	2.55	0.41
14:r:6:LEU:O	14:r:10:LEU:HD23	2.21	0.41
1:A:329:GLU:OE2	17:V:134:LYS:NZ	2.48	0.41
3:C:67:MET:HB3	3:C:88:LEU:HD12	2.02	0.41
22:C:512:CLA:H61	22:C:512:CLA:H93	1.86	0.41
5:E:15:THR:HB	9:J:8:ILE:O	2.20	0.41
13:O:200:ASN:O	13:O:213:GLY:HA3	2.20	0.41
17:V:93:PRO:HA	17:V:101:PHE:CD2	2.55	0.41
5:e:23:HIS:HA	5:e:26:THR:OG1	2.20	0.41
5:e:63:ILE:CG2	5:e:64:PRO:HD2	2.50	0.41
17:v:92:HIS:CE1	17:v:93:PRO:HD2	2.55	0.41
1:A:270:SER:HB3	27:A:410:SQD:O49	2.21	0.41
2:B:433:ASP:OD1	2:B:433:ASP:C	2.64	0.41
2:B:487:SER:OG	2:B:488:PRO:HD2	2.20	0.41
22:C:510:CLA:H193	22:C:510:CLA:HBC3	2.01	0.41
7:H:41:PHE:CE1	7:H:45:ILE:HD11	2.56	0.41
17:V:55:ARG:HD2	36:V:304:HOH:O	2.18	0.41
19:Y:42:ARG:O	19:Y:43:ARG:C	2.62	0.41
1:a:296:ASN:HB3	3:c:401:LEU:HA	2.02	0.41
1:A:328:MET:HE1	4:D:183:LEU:HD13	2.01	0.41
2:B:331:ASN:HB3	2:B:437:LEU:HD12	2.01	0.41
3:C:120:ILE:HD13	3:C:120:ILE:HA	1.90	0.41
3:C:394:GLU:O	3:C:398:HIS:ND1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.50	0.41
13:O:43:LEU:HB3	13:O:81:ILE:HB	2.02	0.41
1:a:188:ALA:HB2	1:a:328:MET:HB2	2.02	0.41
5:e:17:VAL:O	5:e:18:ARG:C	2.63	0.41
7:h:17:GLU:O	7:h:18:TYR:C	2.63	0.41
30:k:102:BCR:H333	30:k:103:BCR:C12	2.50	0.41
11:l:22:LEU:O	11:l:26:VAL:HG23	2.20	0.41
4:D:170:ALA:HB1	4:D:171:PRO:CD	2.50	0.41
5:E:26:THR:O	5:E:30:LEU:HG	2.20	0.41
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.03	0.41
30:b:617:BCR:H20C	30:b:617:BCR:H361	1.92	0.41
3:c:109:PHE:CE2	3:c:113:VAL:CG2	3.04	0.41
3:c:169:GLY:HA2	3:c:241:GLY:HA2	2.03	0.41
5:e:23:HIS:CD2	34:f:101:HEC:NC	2.88	0.41
1:A:339:PHE:HB3	1:A:340:PRO:HD2	2.02	0.41
3:C:140:LEU:O	3:C:143:TYR:N	2.49	0.41
4:D:136:VAL:O	4:D:136:VAL:HG12	2.20	0.41
13:O:243:ILE:HG22	13:O:244:GLU:N	2.36	0.41
1:a:183:MET:HA	22:a:402:CLA:HMD1	2.03	0.41
2:b:348:ASN:HB3	2:b:354:LEU:HD11	2.02	0.41
22:c:504:CLA:H13	22:c:508:CLA:H143	2.03	0.41
30:a:406:BCR:H15C	30:a:406:BCR:H351	1.84	0.41
2:b:478:VAL:O	4:d:139:ARG:HG2	2.20	0.41
16:u:28:ASN:OD1	16:u:54:PRO:HA	2.21	0.41
19:y:17:GLU:HB3	36:y:102:HOH:O	2.19	0.41
1:A:217:SER:HA	4:D:272:LEU:HD12	2.03	0.41
27:A:410:SQD:H122	28:D:411:LHG:C16	2.50	0.41
3:C:443:TRP:CE2	22:C:508:CLA:HMD1	2.56	0.41
1:a:72:LEU:HD23	1:a:72:LEU:HA	1.85	0.41
2:b:124:ARG:HD2	7:h:2:ALA:HB2	2.03	0.41
2:b:228:ALA:HB2	31:b:628:STE:H62	2.02	0.41
22:c:502:CLA:HMB1	22:c:502:CLA:HBB1	2.03	0.41
4:d:167:TRP:O	4:d:168:PHE:C	2.64	0.41
5:e:44:TYR:OH	6:f:43:ILE:HD13	2.20	0.41
7:h:30:LEU:HD12	7:h:34:PHE:HE2	1.86	0.41
19:y:39:LEU:HB3	19:y:46:LEU:CD2	2.48	0.41
6:F:18:VAL:O	6:F:19:ARG:C	2.64	0.41
6:F:34:LEU:HD23	6:F:34:LEU:HA	1.81	0.41
18:X:16:SER:HB3	31:X:101:STE:H92	2.03	0.41
20:Z:34:ASP:HA	20:Z:37:LYS:HG2	2.02	0.41
22:b:603:CLA:C4B	22:b:605:CLA:H93	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:607:CLA:HMB1	22:b:607:CLA:HBB1	2.02	0.41
30:B:617:BCR:H331	30:B:617:BCR:HC8	2.02	0.40
23:D:401:PHO:HBA2	23:D:401:PHO:H3A	1.83	0.40
17:V:55:ARG:NE	36:V:307:HOH:O	2.54	0.40
1:a:36:ILE:O	1:a:39:PRO:HD2	2.21	0.40
1:a:299:GLY:O	1:a:300:PHE:C	2.64	0.40
22:b:605:CLA:CMC	22:b:615:CLA:H43	2.50	0.40
22:c:507:CLA:H192	22:c:507:CLA:H162	1.92	0.40
4:d:52:THR:O	4:d:66:SER:HA	2.20	0.40
3:C:465:PRO:O	3:C:469:MET:HG3	2.20	0.40
2:b:86:ILE:HD12	2:b:86:ILE:O	2.21	0.40
3:c:304:PRO:HG3	3:c:395:TYR:HA	2.02	0.40
3:c:315:MET:HE2	3:c:365:TRP:CZ3	2.56	0.40
4:d:53:THR:HA	4:d:67:TYR:CD2	2.56	0.40
10:k:26:PRO:O	10:k:29:PRO:HD2	2.21	0.40
1:A:15:GLU:OE2	1:A:15:GLU:HA	2.20	0.40
25:A:408:PL9:H251	22:D:403:CLA:H141	2.03	0.40
22:c:509:CLA:H142	22:c:509:CLA:H111	1.93	0.40
4:d:90:LEU:HA	4:d:90:LEU:HD12	1.81	0.40
4:d:196:PHE:HA	4:d:199:MET:HE3	2.03	0.40
4:d:293:LEU:HD23	4:d:293:LEU:HA	2.00	0.40
13:o:164:LEU:HD13	13:o:188:LYS:O	2.21	0.40
14:r:29:LYS:O	14:r:31:VAL:N	2.54	0.40
16:u:27:LEU:HD22	16:u:49:ILE:HG21	2.04	0.40
22:A:403:CLA:H93	22:D:403:CLA:H192	2.04	0.40
2:B:37:MET:O	2:B:41:GLU:HG3	2.20	0.40
4:D:202:ALA:HB2	25:D:407:PL9:H353	2.03	0.40
1:a:133:LEU:HD23	4:d:256:ILE:HG12	2.04	0.40
2:b:317:ASN:HA	2:b:330:MET:HE1	2.04	0.40
22:b:605:CLA:HMA1	22:b:606:CLA:H3A	2.03	0.40
29:A:413:DGD:HD5	2:b:75:TRP:HB3	2.03	0.40
22:B:615:CLA:C15	30:B:618:BCR:H10C	2.52	0.40
22:C:511:CLA:H143	20:Z:20:VAL:HG13	2.03	0.40
4:D:140:PRO:O	4:D:144:ILE:HG13	2.20	0.40
5:E:18:ARG:O	5:E:22[A]:ILE:HG22	2.21	0.40
11:L:8:GLN:NE2	36:L:204:HOH:O	2.54	0.40
13:O:6:THR:HG22	13:O:9:ASP:CG	2.45	0.40
14:R:19:ALA:O	14:R:23:ILE:HG22	2.21	0.40
30:T:101:BCR:H23C	30:T:101:BCR:C38	2.50	0.40
30:T:101:BCR:C23	30:T:101:BCR:C38	3.00	0.40
1:a:65:GLU:OE2	4:d:312:GLU:OE1	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:30:SER:H	3:c:30:SER:HG	1.58	0.40
4:d:101:PHE:CD2	4:d:101:PHE:C	3.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	324 (98%)	8 (2%)	0	100	100
1	a	332/344 (96%)	324 (98%)	8 (2%)	0	100	100
2	B	508/506 (100%)	494 (97%)	14 (3%)	0	100	100
2	b	503/506 (99%)	484 (96%)	16 (3%)	3 (1%)	21	25
3	C	442/461 (96%)	423 (96%)	18 (4%)	1 (0%)	43	53
3	c	451/461 (98%)	437 (97%)	13 (3%)	1 (0%)	43	53
4	D	339/352 (96%)	331 (98%)	8 (2%)	0	100	100
4	d	340/352 (97%)	327 (96%)	13 (4%)	0	100	100
5	E	81/84 (96%)	78 (96%)	2 (2%)	1 (1%)	10	10
5	e	80/84 (95%)	78 (98%)	1 (1%)	1 (1%)	9	9
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	28 (88%)	4 (12%)	0	100	100
7	H	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	55 (90%)	6 (10%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	K	35/46 (76%)	33 (94%)	1 (3%)	1 (3%)	3	2
10	k	35/46 (76%)	32 (91%)	2 (6%)	1 (3%)	3	2
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	227 (93%)	13 (5%)	3 (1%)	10	10
13	o	242/272 (89%)	224 (93%)	15 (6%)	3 (1%)	10	10
14	R	32/41 (78%)	31 (97%)	1 (3%)	0	100	100
14	r	29/41 (71%)	25 (86%)	2 (7%)	2 (7%)	1	0
15	T	28/30 (93%)	28 (100%)	0	0	100	100
15	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	u	95/134 (71%)	89 (94%)	5 (5%)	1 (1%)	11	11
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	21
17	v	135/163 (83%)	128 (95%)	6 (4%)	1 (1%)	18	21
18	X	36/41 (88%)	36 (100%)	0	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	24 (96%)	0	1 (4%)	2	1
19	y	28/46 (61%)	20 (71%)	6 (21%)	2 (7%)	1	0
20	Z	60/62 (97%)	56 (93%)	2 (3%)	2 (3%)	3	1
20	z	60/62 (97%)	53 (88%)	5 (8%)	2 (3%)	3	1
All	All	5240/5688 (92%)	5024 (96%)	189 (4%)	27 (0%)	24	29

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	58	ASN
13	O	62	GLU
17	V	64	PRO
20	Z	31	GLN
20	Z	32	ASP

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Mol	Chain	Res	Type
3	c	416	SER
14	r	31	VAL
16	u	53	ALA
19	y	41	VAL
19	y	43	ARG
20	z	2	THR
19	Y	43	ARG
2	b	294	SER
2	b	295	GLY
2	b	404	GLY
5	E	58	GLN
13	o	61	GLN
14	r	30	GLN
13	O	59	LYS
5	e	83	LEU
13	o	73	ARG
13	o	56	PRO
10	k	38	VAL
20	z	61	VAL
17	v	42	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	260 (96%)	10 (4%)	30	43
1	a	269/280 (96%)	258 (96%)	11 (4%)	27	38
2	B	408/404 (101%)	398 (98%)	10 (2%)	42	58
2	b	402/404 (100%)	386 (96%)	16 (4%)	28	40
3	C	346/362 (96%)	337 (97%)	9 (3%)	40	56
3	c	354/362 (98%)	338 (96%)	16 (4%)	24	35
4	D	276/283 (98%)	267 (97%)	9 (3%)	33	47
4	d	277/283 (98%)	259 (94%)	18 (6%)	15	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	72/73 (99%)	67 (93%)	5 (7%)	14	18
5	e	71/73 (97%)	67 (94%)	4 (6%)	19	25
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	44
6	f	28/39 (72%)	26 (93%)	2 (7%)	13	17
7	H	54/55 (98%)	50 (93%)	4 (7%)	13	15
7	h	53/55 (96%)	46 (87%)	7 (13%)	4	4
8	I	32/34 (94%)	28 (88%)	4 (12%)	4	4
8	i	32/34 (94%)	30 (94%)	2 (6%)	16	21
9	J	24/28 (86%)	22 (92%)	2 (8%)	10	12
9	j	24/28 (86%)	21 (88%)	3 (12%)	4	4
10	K	30/37 (81%)	28 (93%)	2 (7%)	15	19
10	k	30/37 (81%)	23 (77%)	7 (23%)	1	0
11	L	35/35 (100%)	33 (94%)	2 (6%)	18	25
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	5
12	M	28/32 (88%)	25 (89%)	3 (11%)	6	7
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	17
13	O	206/228 (90%)	193 (94%)	13 (6%)	16	21
13	o	207/228 (91%)	197 (95%)	10 (5%)	23	32
14	R	28/33 (85%)	23 (82%)	5 (18%)	2	1
14	r	23/33 (70%)	16 (70%)	7 (30%)	0	0
15	T	26/26 (100%)	24 (92%)	2 (8%)	12	14
15	t	25/26 (96%)	24 (96%)	1 (4%)	28	40
16	U	84/112 (75%)	78 (93%)	6 (7%)	13	17
16	u	84/112 (75%)	79 (94%)	5 (6%)	17	23
17	V	117/138 (85%)	111 (95%)	6 (5%)	21	29
17	v	117/138 (85%)	110 (94%)	7 (6%)	17	23
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	8
18	x	31/34 (91%)	25 (81%)	6 (19%)	1	1
19	Y	19/37 (51%)	16 (84%)	3 (16%)	2	2
19	y	22/37 (60%)	19 (86%)	3 (14%)	3	3
20	Z	52/52 (100%)	44 (85%)	8 (15%)	2	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	z	51/52 (98%)	46 (90%)	5 (10%)	7	8
All	All	4328/4644 (93%)	4085 (94%)	243 (6%)	19	25

All (243) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	210	LEU
1	A	228	THR
1	A	229	GLU
1	A	231	GLU
1	A	243	GLU
1	A	244	GLU
1	A	248	ILE
1	A	270	SER
1	A	307	ILE
2	B	63	LEU
2	B	98	LEU
2	B	101	ILE
2	B	127	ARG
2	B	138	MET
2	B	289	GLN
2	B	297	THR
2	B	350	GLU
2	B	353	GLU
2	B	371	THR
3	C	120	ILE
3	C	141	GLU
3	C	201	ASN
3	C	279	LEU
3	C	289	PHE
3	C	315	MET
3	C	355	THR
3	C	386	PRO
3	C	416	SER
4	D	165	SER
4	D	224	GLN
4	D	238	THR
4	D	248	THR
4	D	259	ILE
4	D	262	SER
4	D	329	MET

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Mol	Chain	Res	Type
4	D	343	GLU
4	D	345	VAL
5	E	16	SER
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	32	ILE
5	E	61	ARG
6	F	25	THR
7	H	20	LYS
7	H	30	LEU
7	H	56	ASP
7	H	65	LEU
8	I	2	GLU
8	I	4	LEU
8	I	7	THR
8	I	36	ASP
9	J	8	ILE
9	J	24	ILE
10	K	13	GLU
10	K	25	LEU
11	L	7	ARG
11	L	11	GLU
12	M	16	LEU
12	M	20	VAL
12	M	25	LEU
13	O	3	GLN
13	O	36	GLN
13	O	39	ARG
13	O	78	LEU
13	O	89	SER
13	O	97	GLU
13	O	107	THR
13	O	118	LEU
13	O	191	SER
13	O	198	SER
13	O	214	THR
13	O	218	GLU
13	O	225	MET
14	R	6	LEU
14	R	10	LEU
14	R	21	ARG
14	R	22	ASN

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Mol	Chain	Res	Type
14	R	29	LYS
15	T	25	GLU
15	T	29	ILE
16	U	10	VAL
16	U	39	ARG
16	U	51	LYS
16	U	61	VAL
16	U	63	ASN
16	U	67	LEU
17	V	3	LEU
17	V	7	VAL
17	V	17	LYS
17	V	19	ILE
17	V	42	VAL
17	V	99	ASP
18	X	3	ILE
18	X	29	ILE
18	X	37	VAL
19	Y	23	THR
19	Y	34	MET
19	Y	41	VAL
20	Z	3	ILE
20	Z	4	LEU
20	Z	7	LEU
20	Z	15	LEU
20	Z	17	PHE
20	Z	31	GLN
20	Z	35	ARG
20	Z	46	LEU
1	a	28	LEU
1	a	42	LEU
1	a	159	LEU
1	a	200	LEU
1	a	223	LEU
1	a	226	GLU
1	a	229	GLU
1	a	230	THR
1	a	245	THR
1	a	248	ILE
1	a	288	LEU
2	b	13	ILE
2	b	83	GLU

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Mol	Chain	Res	Type
2	b	98	LEU
2	b	128	THR
2	b	137	LYS
2	b	149	LEU
2	b	161	LEU
2	b	236	THR
2	b	286	ARG
2	b	298	LEU
2	b	362	PHE
2	b	425	ILE
2	b	480	SER
2	b	485	GLU
2	b	491	VAL
2	b	506	ARG
3	c	24	THR
3	c	29	GLU
3	c	30	SER
3	c	72	LEU
3	c	124	VAL
3	c	125	LEU
3	c	135	ARG
3	c	144	SER
3	c	165	LEU
3	c	200	THR
3	c	221	GLU
3	c	255	THR
3	c	279	LEU
3	c	289	PHE
3	c	315	MET
3	c	355	THR
4	d	12	ARG
4	d	25	ASP
4	d	28	VAL
4	d	90	LEU
4	d	103	ARG
4	d	150	ILE
4	d	182	LEU
4	d	227[A]	GLU
4	d	227[B]	GLU
4	d	230	SER
4	d	233	ARG
4	d	256	ILE

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Mol	Chain	Res	Type
4	d	259	ILE
4	d	272	LEU
4	d	291	LEU
4	d	293	LEU
4	d	307	GLU
4	d	321	LEU
5	e	4	THR
5	e	65	LEU
5	e	75	GLN
5	e	84	LYS
6	f	15	ILE
6	f	28	VAL
7	h	7	LEU
7	h	12	ARG
7	h	27	THR
7	h	30	LEU
7	h	37	LEU
7	h	39	LEU
7	h	43	LEU
8	i	6	ILE
8	i	36	ASP
9	j	7	ARG
9	j	13	VAL
9	j	21	VAL
10	k	10	LYS
10	k	13	GLU
10	k	17	ILE
10	k	25	LEU
10	k	30	VAL
10	k	35	LEU
10	k	46	ARG
11	l	2	GLU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
12	m	16	LEU
13	o	49	THR
13	o	53	LYS
13	o	64	GLU
13	o	87	VAL
13	o	89	SER

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Mol	Chain	Res	Type
13	o	118	LEU
13	o	135	SER
13	o	191	SER
13	o	198	SER
13	o	207	ARG
14	r	6	LEU
14	r	7	VAL
14	r	9	LEU
14	r	10	LEU
14	r	12	VAL
14	r	13	LEU
14	r	24	LEU
15	t	29	ILE
16	u	10	VAL
16	u	15	GLU
16	u	23	GLU
16	u	51	LYS
16	u	80	GLU
17	v	19	ILE
17	v	22	THR
17	v	52	LEU
17	v	90	GLU
17	v	107	LEU
17	v	108	THR
17	v	112	LEU
18	x	2	THR
18	x	7	LEU
18	x	8	LYS
18	x	14	LEU
18	x	15	LEU
18	x	21	LEU
19	y	19	ILE
19	y	23	THR
19	y	30	ILE
20	z	1	MET
20	z	7	LEU
20	z	20	VAL
20	z	32	ASP
20	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	165	GLN
1	A	199	GLN
1	A	261	GLN
1	A	338	ASN
2	B	409	GLN
3	C	327	ASN
3	C	385	GLN
5	E	60	GLN
12	M	5	GLN
13	O	3	GLN
13	O	36	GLN
13	O	88	ASN
13	O	155	ASN
16	U	37	GLN
16	U	78	ASN
17	V	78	ASN
18	X	38	GLN
19	Y	21	GLN
19	Y	45	ASN
20	Z	6	GLN
20	Z	31	GLN
1	a	165	GLN
1	a	181	ASN
1	a	199	GLN
1	a	234	ASN
2	b	409	GLN
3	c	327	ASN
3	c	378	ASN
7	h	59	ASN
8	i	31	ASN
13	o	61	GLN
13	o	124	ASN
13	o	130	GLN
13	o	196	GLN
13	o	219	GLN
14	r	30	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
15	FME	t	1	15	8,9,10	1.59	1 (12%)	8,9,11	1.12	0
8	FME	I	1	8	8,9,10	1.08	0	8,9,11	0.59	0
12	FME	m	1	12	8,9,10	0.93	0	8,9,11	1.56	2 (25%)
8	FME	i	1	8	8,9,10	1.29	1 (12%)	8,9,11	1.21	1 (12%)
12	FME	M	1	12	8,9,10	1.20	1 (12%)	8,9,11	1.07	1 (12%)
15	FME	T	1	15	8,9,10	1.13	1 (12%)	8,9,11	0.89	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FME	t	1	15	-	4/7/9/11	-
8	FME	I	1	8	-	3/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
15	FME	T	1	15	-	4/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-4.16	1.40	1.46
8	i	1	FME	CA-N	-2.82	1.42	1.46
12	M	1	FME	CA-N	-2.72	1.42	1.46
15	T	1	FME	CA-N	-2.21	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	m	1	FME	CA-N-CN	2.85	127.20	122.82
12	m	1	FME	CB-CA-N	2.68	115.40	110.52
8	i	1	FME	CA-N-CN	-2.39	119.14	122.82
12	M	1	FME	CA-N-CN	-2.06	119.65	122.82

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	1	FME	O-C-CA-CB
15	t	1	FME	O-C-CA-CB
15	t	1	FME	CB-CG-SD-CE
15	T	1	FME	N-CA-CB-CG
15	T	1	FME	CB-CG-SD-CE
15	T	1	FME	C-CA-CB-CG
15	t	1	FME	C-CA-CB-CG
8	I	1	FME	N-CA-CB-CG
15	t	1	FME	N-CA-CB-CG
8	I	1	FME	CB-CG-SD-CE
8	i	1	FME	CB-CG-SD-CE
12	m	1	FME	CB-CG-SD-CE
8	I	1	FME	CB-CA-N-CN
8	i	1	FME	CB-CA-N-CN
12	M	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 190 ligands modelled in this entry, 7 are monoatomic - leaving 183 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	606	2	69,73,73	1.64	10 (14%)	82,113,113	1.48	10 (12%)
31	STE	I	102	-	14,14,19	0.71	0	13,13,19	0.41	0
23	PHO	A	404	-	58,69,69	1.76	10 (17%)	55,99,99	1.76	13 (23%)
29	DGD	C	517	-	63,63,67	1.25	9 (14%)	77,77,81	1.39	10 (12%)
31	STE	b	625	-	14,14,19	0.40	0	13,13,19	0.92	0
30	BCR	B	618	-	41,41,41	1.26	3 (7%)	56,56,56	1.61	11 (19%)
30	BCR	T	101	-	41,41,41	1.11	4 (9%)	56,56,56	1.29	5 (8%)
22	CLA	b	607	36	69,73,73	1.35	12 (17%)	82,113,113	1.16	5 (6%)
28	LHG	a	411	-	41,41,48	1.18	5 (12%)	44,47,54	1.26	4 (9%)
30	BCR	K	102	-	41,41,41	1.20	2 (4%)	56,56,56	1.35	9 (16%)
30	BCR	H	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.25	6 (10%)
28	LHG	d	408	-	48,48,48	0.80	2 (4%)	51,54,54	1.14	3 (5%)
31	STE	b	621	-	19,19,19	0.75	0	19,19,19	0.95	1 (5%)
30	BCR	K	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.53	11 (19%)
22	CLA	B	608	2	69,73,73	1.21	7 (10%)	82,113,113	1.45	13 (15%)
31	STE	Z	101	-	7,7,19	0.56	0	6,6,19	0.27	0
26	LMG	D	408	-	51,51,55	1.19	4 (7%)	59,59,63	1.35	6 (10%)
31	STE	k	104	-	11,11,19	0.94	0	11,11,19	0.87	0
31	STE	M	103	-	9,9,19	0.77	0	8,8,19	0.40	0
22	CLA	a	402	1	69,73,73	1.32	9 (13%)	82,113,113	1.50	10 (12%)
28	LHG	L	102	-	48,48,48	0.91	2 (4%)	51,54,54	1.19	4 (7%)
26	LMG	m	101	-	51,51,55	1.26	4 (7%)	59,59,63	1.50	8 (13%)
23	PHO	d	401	-	58,69,69	2.27	11 (18%)	55,99,99	1.82	11 (20%)
30	BCR	b	618	-	41,41,41	1.51	4 (9%)	56,56,56	1.33	10 (17%)
22	CLA	b	611	2	69,73,73	1.32	10 (14%)	82,113,113	1.47	15 (18%)
22	CLA	B	615	2	64,68,73	1.55	10 (15%)	76,107,113	1.45	8 (10%)
22	CLA	C	503	3	69,73,73	1.43	12 (17%)	82,113,113	1.73	12 (14%)
31	STE	t	104	-	9,9,19	0.60	0	8,8,19	0.37	0
22	CLA	D	403	4	69,73,73	1.31	6 (8%)	82,113,113	1.19	7 (8%)
34	HEC	F	101	5,6	50,50,50	1.74	6 (12%)	68,82,82	1.39	8 (11%)
22	CLA	B	603	2	69,73,73	1.32	9 (13%)	82,113,113	1.67	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	606	36	69,73,73	1.40	10 (14%)	82,113,113	1.34	3 (3%)
22	CLA	b	614	2	69,73,73	1.61	12 (17%)	82,113,113	1.41	12 (14%)
22	CLA	A	405	1	58,62,73	1.30	7 (12%)	68,99,113	1.53	10 (14%)
30	BCR	d	406	-	41,41,41	1.10	2 (4%)	56,56,56	1.42	9 (16%)
22	CLA	C	511	3	69,73,73	1.42	11 (15%)	82,113,113	1.48	4 (4%)
26	LMG	d	410	-	44,44,55	1.21	5 (11%)	52,52,63	1.26	6 (11%)
22	CLA	b	602	2	69,73,73	1.56	10 (14%)	82,113,113	1.52	12 (14%)
28	LHG	A	411	-	48,48,48	1.03	3 (6%)	51,54,54	1.24	5 (9%)
22	CLA	B	607	2	69,73,73	1.48	9 (13%)	82,113,113	1.13	8 (9%)
26	LMG	D	412	-	31,31,55	1.26	3 (9%)	33,33,63	1.13	2 (6%)
29	DGD	C	518	-	63,63,67	1.12	6 (9%)	77,77,81	1.52	11 (14%)
25	PL9	d	407	-	55,55,55	1.60	11 (20%)	68,69,69	1.51	15 (22%)
31	STE	x	102	-	19,19,19	0.78	0	19,19,19	0.96	2 (10%)
22	CLA	c	511	3	69,73,73	1.52	8 (11%)	82,113,113	1.48	10 (12%)
27	SQD	f	102	-	39,41,54	1.14	4 (10%)	49,52,65	1.91	13 (26%)
30	BCR	B	617	-	41,41,41	1.10	1 (2%)	56,56,56	1.43	11 (19%)
22	CLA	b	608	2	69,73,73	1.09	8 (11%)	82,113,113	1.41	10 (12%)
22	CLA	C	505	3	69,73,73	1.23	8 (11%)	82,113,113	1.28	9 (10%)
22	CLA	d	403	4	69,73,73	1.51	10 (14%)	82,113,113	1.32	7 (8%)
27	SQD	t	102	-	35,35,54	1.22	3 (8%)	37,37,65	1.48	4 (10%)
22	CLA	a	405	1	69,73,73	1.45	8 (11%)	82,113,113	1.31	9 (10%)
22	CLA	b	604	2	69,73,73	1.26	7 (10%)	82,113,113	1.50	13 (15%)
25	PL9	a	409	-	55,55,55	1.14	4 (7%)	68,69,69	1.52	13 (19%)
31	STE	X	101	-	19,19,19	0.64	0	19,19,19	1.23	2 (10%)
22	CLA	d	405	4	69,73,73	1.68	12 (17%)	82,113,113	1.17	8 (9%)
22	CLA	c	506	3	69,73,73	1.66	7 (10%)	82,113,113	1.47	15 (18%)
25	PL9	A	408	-	55,55,55	1.54	5 (9%)	68,69,69	1.50	12 (17%)
22	CLA	b	601	36	69,73,73	1.31	11 (15%)	82,113,113	1.48	10 (12%)
31	STE	J	101	-	11,11,19	0.69	0	11,11,19	1.29	1 (9%)
30	BCR	b	617	-	41,41,41	1.09	3 (7%)	56,56,56	1.38	9 (16%)
30	BCR	k	102	-	41,41,41	1.08	3 (7%)	56,56,56	1.18	4 (7%)
31	STE	b	629	-	19,19,19	0.78	1 (5%)	19,19,19	0.92	0
22	CLA	c	502	3	69,73,73	1.45	10 (14%)	82,113,113	1.36	13 (15%)
22	CLA	B	609	36	69,73,73	1.36	10 (14%)	82,113,113	1.55	10 (12%)
22	CLA	c	503	3	69,73,73	1.20	8 (11%)	82,113,113	1.28	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	611	2	69,73,73	1.30	10 (14%)	82,113,113	1.31	9 (10%)
30	BCR	k	103	-	41,41,41	1.11	3 (7%)	56,56,56	1.33	5 (8%)
28	LHG	D	413	-	48,48,48	1.05	3 (6%)	51,54,54	1.42	7 (13%)
22	CLA	c	507	36	69,73,73	1.85	11 (15%)	82,113,113	1.45	10 (12%)
28	LHG	b	623	-	48,48,48	0.96	2 (4%)	51,54,54	1.26	4 (7%)
30	BCR	D	406	-	41,41,41	1.14	4 (9%)	56,56,56	1.33	6 (10%)
31	STE	B	623	-	17,17,19	0.77	0	17,17,19	0.94	0
31	STE	c	519	-	19,19,19	0.78	1 (5%)	19,19,19	0.84	0
30	BCR	k	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.44	11 (19%)
22	CLA	B	604	2	69,73,73	1.00	5 (7%)	82,113,113	1.40	9 (10%)
22	CLA	B	610	2	69,73,73	1.50	11 (15%)	82,113,113	1.62	13 (15%)
22	CLA	c	504	36	64,68,73	1.27	9 (14%)	76,107,113	1.24	12 (15%)
22	CLA	b	613	2	69,73,73	1.52	9 (13%)	82,113,113	1.43	9 (10%)
22	CLA	D	405	4	69,73,73	1.81	14 (20%)	82,113,113	1.12	5 (6%)
30	BCR	t	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.45	12 (21%)
29	DGD	c	515	-	63,63,67	1.34	8 (12%)	77,77,81	1.44	13 (16%)
28	LHG	D	411	-	46,46,48	1.08	3 (6%)	49,52,54	1.24	5 (10%)
26	LMG	Y	101	-	48,48,55	1.11	7 (14%)	56,56,63	1.26	6 (10%)
26	LMG	B	620	-	26,26,55	1.44	5 (19%)	26,26,63	1.07	2 (7%)
29	DGD	H	103	-	63,63,67	1.34	8 (12%)	77,77,81	1.58	13 (16%)
30	BCR	b	619	-	41,41,41	1.12	2 (4%)	56,56,56	1.37	9 (16%)
32	OEX	a	415	3,36,1	0,14,14	-	-	-	-	-
22	CLA	b	612	2	69,73,73	1.32	9 (13%)	82,113,113	1.46	10 (12%)
34	HEC	V	201	17	50,50,50	1.61	3 (6%)	68,82,82	1.46	13 (19%)
23	PHO	a	404	-	58,69,69	1.92	10 (17%)	55,99,99	1.71	11 (20%)
22	CLA	C	504	36	63,67,73	1.34	8 (12%)	74,105,113	1.35	11 (14%)
31	STE	L	103	-	11,11,19	0.77	0	11,11,19	1.70	2 (18%)
34	HEC	f	101	5,6	50,50,50	1.71	6 (12%)	68,82,82	1.59	14 (20%)
26	LMG	c	520	-	48,48,55	1.07	3 (6%)	56,56,63	1.30	7 (12%)
33	BCT	D	402	21	3,3,3	0.97	0	2,3,3	3.95	2 (100%)
27	SQD	B	621	-	52,54,54	1.03	3 (5%)	62,65,65	1.89	15 (24%)
28	LHG	d	409	-	38,38,48	1.08	4 (10%)	41,44,54	1.23	5 (12%)
26	LMG	M	101	-	51,51,55	1.10	4 (7%)	59,59,63	1.40	8 (13%)
31	STE	M	102	-	14,14,19	0.92	0	14,14,19	1.01	1 (7%)
22	CLA	c	501	3	69,73,73	1.71	10 (14%)	82,113,113	1.55	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PHO	D	401	-	58,69,69	2.03	9 (15%)	55,99,99	1.58	10 (18%)
27	SQD	L	101	-	47,49,54	1.00	2 (4%)	57,60,65	2.32	18 (31%)
30	BCR	a	406	-	41,41,41	1.11	3 (7%)	56,56,56	1.53	13 (23%)
31	STE	B	622	-	11,11,19	0.79	0	11,11,19	1.39	1 (9%)
31	STE	C	521	-	11,11,19	0.68	0	11,11,19	1.43	2 (18%)
29	DGD	h	101	-	63,63,67	1.04	4 (6%)	77,77,81	1.46	14 (18%)
22	CLA	B	602	2	69,73,73	1.16	7 (10%)	82,113,113	1.48	14 (17%)
31	STE	d	411	-	16,16,19	0.80	0	16,16,19	0.98	1 (6%)
22	CLA	C	502	3	69,73,73	1.62	8 (11%)	82,113,113	1.38	10 (12%)
31	STE	b	627	-	9,9,19	0.61	0	8,8,19	0.46	0
31	STE	M	104	-	17,17,19	0.43	0	16,16,19	0.85	0
22	CLA	C	506	3	69,73,73	1.66	12 (17%)	82,113,113	1.34	9 (10%)
22	CLA	A	402	1	69,73,73	1.19	6 (8%)	82,113,113	1.51	16 (19%)
22	CLA	C	510	3	69,73,73	1.42	12 (17%)	82,113,113	1.67	9 (10%)
30	BCR	I	101	-	41,41,41	1.20	5 (12%)	56,56,56	1.58	12 (21%)
31	STE	C	520	-	15,15,19	0.59	0	14,14,19	0.53	0
22	CLA	D	404	36	69,73,73	1.47	10 (14%)	82,113,113	1.21	8 (9%)
31	STE	H	104	-	17,17,19	0.48	0	16,16,19	0.64	0
22	CLA	A	403	36	69,73,73	1.45	10 (14%)	82,113,113	1.38	10 (12%)
22	CLA	B	601	2	69,73,73	1.51	10 (14%)	82,113,113	1.33	13 (15%)
27	SQD	D	409	-	34,36,54	1.08	2 (5%)	42,45,65	1.84	11 (26%)
31	STE	j	101	-	11,11,19	1.03	1 (9%)	11,11,19	0.73	0
34	HEC	v	201	17	50,50,50	1.60	6 (12%)	68,82,82	1.51	12 (17%)
31	STE	b	628	-	13,13,19	0.60	0	12,12,19	0.37	0
27	SQD	a	410	-	52,54,54	1.04	3 (5%)	62,65,65	1.73	14 (22%)
22	CLA	b	615	2	69,73,73	2.18	12 (17%)	82,113,113	1.39	9 (10%)
31	STE	B	625	-	11,11,19	0.83	0	11,11,19	1.50	3 (27%)
22	CLA	C	508	3	69,73,73	1.50	9 (13%)	82,113,113	1.36	14 (17%)
22	CLA	b	605	2	69,73,73	1.23	12 (17%)	82,113,113	1.53	13 (15%)
28	LHG	D	410	-	48,48,48	1.00	3 (6%)	51,54,54	1.24	5 (9%)
22	CLA	C	513	3	69,73,73	1.22	10 (14%)	82,113,113	1.49	11 (13%)
22	CLA	c	509	3	69,73,73	1.35	8 (11%)	82,113,113	1.48	11 (13%)
22	CLA	b	616	2	64,68,73	1.19	7 (10%)	76,107,113	1.51	10 (13%)
22	CLA	a	403	36	69,73,73	1.31	10 (14%)	82,113,113	1.36	11 (13%)
22	CLA	b	609	2	69,73,73	1.55	10 (14%)	82,113,113	1.42	11 (13%)
31	STE	B	619	-	16,16,19	0.88	1 (6%)	16,16,19	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	STE	a	413	-	14,14,19	0.49	0	13,13,19	0.66	0
22	CLA	C	512	3	69,73,73	1.28	8 (11%)	82,113,113	1.42	10 (12%)
26	LMG	a	414	-	55,55,55	1.53	9 (16%)	63,63,63	1.29	8 (12%)
30	BCR	C	515	-	41,41,41	1.03	2 (4%)	56,56,56	1.30	8 (14%)
30	BCR	c	514	-	41,41,41	1.19	3 (7%)	56,56,56	1.61	12 (21%)
31	STE	b	626	-	19,19,19	0.86	0	19,19,19	0.52	0
22	CLA	B	605	2	69,73,73	1.74	9 (13%)	82,113,113	1.34	9 (10%)
29	DGD	c	516	-	63,63,67	1.09	7 (11%)	77,77,81	1.54	17 (22%)
22	CLA	c	508	3	68,72,73	1.29	9 (13%)	80,111,113	1.32	10 (12%)
30	BCR	x	101	-	41,41,41	1.05	3 (7%)	56,56,56	1.47	11 (19%)
32	OEX	C	522	3,36,1	0,14,14	-	-	-	-	-
33	BCT	d	402	21	3,3,3	1.10	0	2,3,3	3.08	1 (50%)
22	CLA	H	101	36	69,73,73	1.55	8 (11%)	82,113,113	1.43	6 (7%)
28	LHG	l	101	-	48,48,48	0.92	3 (6%)	51,54,54	1.12	2 (3%)
26	LMG	c	521	-	49,49,55	1.12	6 (12%)	57,57,63	1.34	8 (14%)
30	BCR	B	616	-	41,41,41	1.10	3 (7%)	56,56,56	1.42	8 (14%)
22	CLA	C	501	3	69,73,73	1.58	10 (14%)	82,113,113	1.55	10 (12%)
31	STE	b	624	-	15,15,19	0.88	0	15,15,19	0.90	0
22	CLA	B	614	2	69,73,73	1.32	10 (14%)	82,113,113	1.42	10 (12%)
29	DGD	C	516	-	63,63,67	1.40	9 (14%)	77,77,81	1.38	11 (14%)
22	CLA	B	612	2	69,73,73	1.93	10 (14%)	82,113,113	1.23	7 (8%)
22	CLA	b	603	2	69,73,73	1.54	7 (10%)	82,113,113	1.76	15 (18%)
27	SQD	A	410	-	50,52,54	1.13	4 (8%)	60,63,65	2.02	17 (28%)
31	STE	C	519	-	11,11,19	1.03	0	11,11,19	1.41	2 (18%)
26	LMG	b	622	-	55,55,55	1.17	5 (9%)	63,63,63	1.46	5 (7%)
22	CLA	c	513	3	69,73,73	1.28	9 (13%)	82,113,113	1.26	6 (7%)
30	BCR	C	514	-	41,41,41	1.28	2 (4%)	56,56,56	1.54	13 (23%)
29	DGD	A	413	-	67,67,67	1.41	10 (14%)	81,81,81	1.32	13 (16%)
22	CLA	c	505	3	69,73,73	1.11	6 (8%)	82,113,113	1.36	8 (9%)
22	CLA	d	404	36	69,73,73	1.49	7 (10%)	82,113,113	1.66	14 (17%)
26	LMG	A	409	-	48,48,55	1.17	5 (10%)	56,56,63	1.42	8 (14%)
22	CLA	C	507	36	69,73,73	1.21	6 (8%)	82,113,113	1.41	6 (7%)
22	CLA	B	613	2	69,73,73	1.20	5 (7%)	82,113,113	1.30	11 (13%)
22	CLA	c	510	3	69,73,73	1.10	7 (10%)	82,113,113	1.37	8 (9%)
29	DGD	c	517	-	63,63,67	1.22	9 (14%)	77,77,81	1.37	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	512	3	69,73,73	1.59	13 (18%)	82,113,113	1.45	9 (10%)
31	STE	t	103	-	13,13,19	0.91	0	13,13,19	1.09	2 (15%)
22	CLA	C	509	3	69,73,73	1.29	10 (14%)	82,113,113	1.30	10 (12%)
31	STE	R	101	-	11,11,19	0.76	0	11,11,19	1.09	1 (9%)
31	STE	b	620	-	15,15,19	0.57	0	14,14,19	0.72	0
27	SQD	A	412	-	38,38,54	1.10	2 (5%)	40,40,65	1.41	5 (12%)
31	STE	a	412	-	11,11,19	0.84	0	11,11,19	0.95	0
22	CLA	b	610	36	69,73,73	1.81	9 (13%)	82,113,113	1.36	10 (12%)
25	PL9	D	407	-	55,55,55	1.62	12 (21%)	68,69,69	1.64	15 (22%)
31	STE	B	624	-	15,15,19	0.50	0	14,14,19	0.84	0
26	LMG	c	518	-	37,37,55	1.43	8 (21%)	45,45,63	1.32	5 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	606	2	-	8/39/115/115	-
31	STE	I	102	-	-	5/12/12/17	-
23	PHO	A	404	-	-	6/37/103/103	0/5/6/6
29	DGD	C	517	-	-	21/51/91/95	0/2/2/2
31	STE	b	625	-	-	7/12/12/17	-
30	BCR	B	618	-	-	9/29/63/63	0/2/2/2
30	BCR	T	101	-	-	12/29/63/63	0/2/2/2
22	CLA	b	607	36	-	15/39/115/115	-
28	LHG	a	411	-	-	25/46/46/53	-
30	BCR	K	102	-	-	11/29/63/63	0/2/2/2
30	BCR	H	102	-	-	10/29/63/63	0/2/2/2
28	LHG	d	408	-	-	21/53/53/53	-
31	STE	b	621	-	-	10/17/17/17	-
30	BCR	K	101	-	-	12/29/63/63	0/2/2/2
22	CLA	B	608	2	-	6/39/115/115	-
31	STE	Z	101	-	-	4/5/5/17	-
26	LMG	D	408	-	-	17/46/66/70	0/1/1/1
31	STE	k	104	-	-	5/9/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	STE	M	103	-	-	2/7/7/17	-
22	CLA	a	402	1	-	1/39/115/115	-
28	LHG	L	102	-	-	23/53/53/53	-
26	LMG	m	101	-	-	18/46/66/70	0/1/1/1
23	PHO	d	401	-	-	6/37/103/103	0/5/6/6
30	BCR	b	618	-	-	4/29/63/63	0/2/2/2
22	CLA	b	611	2	-	7/39/115/115	-
22	CLA	B	615	2	-	7/33/109/115	-
22	CLA	C	503	3	-	4/39/115/115	-
31	STE	t	104	-	-	3/7/7/17	-
22	CLA	D	403	4	-	6/39/115/115	-
34	HEC	F	101	5,6	1/1/7/7	6/14/54/54	-
22	CLA	B	603	2	-	13/39/115/115	-
22	CLA	B	606	36	-	17/39/115/115	-
22	CLA	b	614	2	-	17/39/115/115	-
22	CLA	A	405	1	-	3/26/102/115	-
30	BCR	d	406	-	-	7/29/63/63	0/2/2/2
22	CLA	C	511	3	-	7/39/115/115	-
26	LMG	d	410	-	-	10/39/59/70	0/1/1/1
22	CLA	b	602	2	-	12/39/115/115	-
28	LHG	A	411	-	-	23/53/53/53	-
22	CLA	B	607	2	-	8/39/115/115	-
26	LMG	D	412	-	-	19/33/33/70	-
29	DGD	C	518	-	-	15/51/91/95	0/2/2/2
25	PL9	d	407	-	-	18/53/73/73	0/1/1/1
31	STE	x	102	-	-	11/17/17/17	-
22	CLA	c	511	3	-	9/39/115/115	-
27	SQD	f	102	-	-	14/36/56/69	0/1/1/1
30	BCR	B	617	-	-	10/29/63/63	0/2/2/2
22	CLA	b	608	2	-	6/39/115/115	-
22	CLA	C	505	3	-	7/39/115/115	-
22	CLA	d	403	4	-	10/39/115/115	-
27	SQD	t	102	-	-	12/37/37/69	-
22	CLA	a	405	1	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	604	2	-	12/39/115/115	-
25	PL9	a	409	-	-	26/53/73/73	0/1/1/1
31	STE	X	101	-	-	10/17/17/17	-
22	CLA	d	405	4	-	7/39/115/115	-
22	CLA	c	506	3	-	12/39/115/115	-
25	PL9	A	408	-	-	21/53/73/73	0/1/1/1
22	CLA	b	601	36	-	23/39/115/115	-
31	STE	J	101	-	-	5/9/9/17	-
30	BCR	b	617	-	-	9/29/63/63	0/2/2/2
30	BCR	k	102	-	-	15/29/63/63	0/2/2/2
31	STE	b	629	-	-	6/17/17/17	-
22	CLA	c	502	3	-	12/39/115/115	-
22	CLA	B	609	36	-	7/39/115/115	-
22	CLA	c	503	3	-	9/39/115/115	-
22	CLA	B	611	2	-	6/39/115/115	-
30	BCR	k	103	-	-	6/29/63/63	0/2/2/2
28	LHG	D	413	-	-	20/53/53/53	-
22	CLA	c	507	36	-	12/39/115/115	-
28	LHG	b	623	-	-	26/53/53/53	-
30	BCR	D	406	-	-	8/29/63/63	0/2/2/2
31	STE	B	623	-	-	11/15/15/17	-
31	STE	c	519	-	-	7/17/17/17	-
30	BCR	k	101	-	-	10/29/63/63	0/2/2/2
22	CLA	B	604	2	-	11/39/115/115	-
22	CLA	B	610	2	-	6/39/115/115	-
22	CLA	c	504	36	-	4/33/109/115	-
22	CLA	b	613	2	-	10/39/115/115	-
22	CLA	D	405	4	-	13/39/115/115	-
30	BCR	t	101	-	-	13/29/63/63	0/2/2/2
29	DGD	c	515	-	-	22/51/91/95	0/2/2/2
28	LHG	D	411	-	-	21/51/51/53	-
26	LMG	Y	101	-	-	22/43/63/70	0/1/1/1
26	LMG	B	620	-	-	8/22/22/70	-
29	DGD	H	103	-	-	17/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	b	619	-	-	3/29/63/63	0/2/2/2
22	CLA	b	612	2	-	6/39/115/115	-
34	HEC	V	201	17	1/1/7/7	6/14/54/54	-
23	PHO	a	404	-	-	1/37/103/103	0/5/6/6
22	CLA	C	504	36	-	6/32/108/115	-
34	HEC	f	101	5,6	1/1/7/7	6/14/54/54	-
31	STE	L	103	-	-	5/9/9/17	-
26	LMG	c	520	-	-	20/43/63/70	0/1/1/1
27	SQD	B	621	-	-	24/49/69/69	0/1/1/1
28	LHG	d	409	-	-	13/43/43/53	-
26	LMG	M	101	-	-	17/46/66/70	0/1/1/1
31	STE	M	102	-	-	6/12/12/17	-
22	CLA	c	501	3	-	5/39/115/115	-
23	PHO	D	401	-	-	4/37/103/103	0/5/6/6
27	SQD	L	101	-	-	26/44/64/69	0/1/1/1
30	BCR	a	406	-	-	2/29/63/63	0/2/2/2
31	STE	B	622	-	-	5/9/9/17	-
31	STE	C	521	-	-	2/9/9/17	-
29	DGD	h	101	-	-	16/51/91/95	0/2/2/2
22	CLA	B	602	2	-	11/39/115/115	-
31	STE	d	411	-	-	9/14/14/17	-
22	CLA	C	502	3	-	9/39/115/115	-
31	STE	b	627	-	-	5/7/7/17	-
31	STE	M	104	-	-	9/15/15/17	-
22	CLA	C	506	3	-	21/39/115/115	-
22	CLA	A	402	1	-	3/39/115/115	-
22	CLA	C	510	3	-	12/39/115/115	-
30	BCR	I	101	-	-	7/29/63/63	0/2/2/2
31	STE	C	520	-	-	4/13/13/17	-
22	CLA	D	404	36	-	7/39/115/115	-
31	STE	H	104	-	-	9/15/15/17	-
22	CLA	A	403	36	-	8/39/115/115	-
22	CLA	B	601	2	-	7/39/115/115	-
27	SQD	D	409	-	-	14/28/48/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	STE	j	101	-	-	2/9/9/17	-
34	HEC	v	201	17	1/1/7/7	5/14/54/54	-
31	STE	b	628	-	-	7/11/11/17	-
27	SQD	a	410	-	-	22/49/69/69	0/1/1/1
22	CLA	b	615	2	-	13/39/115/115	-
31	STE	B	625	-	-	4/9/9/17	-
22	CLA	C	508	3	-	10/39/115/115	-
22	CLA	b	605	2	-	13/39/115/115	-
28	LHG	D	410	-	-	22/53/53/53	-
22	CLA	C	513	3	-	7/39/115/115	-
22	CLA	c	509	3	-	6/39/115/115	-
22	CLA	b	616	2	-	5/33/109/115	-
22	CLA	a	403	36	-	10/39/115/115	-
22	CLA	b	609	2	-	9/39/115/115	-
31	STE	B	619	-	-	6/14/14/17	-
31	STE	a	413	-	-	9/12/12/17	-
22	CLA	C	512	3	-	11/39/115/115	-
26	LMG	a	414	-	-	31/50/70/70	0/1/1/1
30	BCR	C	515	-	-	11/29/63/63	0/2/2/2
30	BCR	c	514	-	-	7/29/63/63	0/2/2/2
31	STE	b	626	-	-	9/17/17/17	-
22	CLA	B	605	2	-	12/39/115/115	-
29	DGD	c	516	-	-	17/51/91/95	0/2/2/2
22	CLA	c	508	3	-	12/38/114/115	-
30	BCR	x	101	-	-	7/29/63/63	0/2/2/2
22	CLA	H	101	36	-	18/39/115/115	-
28	LHG	l	101	-	-	17/53/53/53	-
26	LMG	c	521	-	-	24/44/64/70	0/1/1/1
30	BCR	B	616	-	-	7/29/63/63	0/2/2/2
22	CLA	C	501	3	-	5/39/115/115	-
31	STE	b	624	-	-	10/13/13/17	-
22	CLA	B	614	2	-	9/39/115/115	-
29	DGD	C	516	-	-	18/51/91/95	0/2/2/2
22	CLA	B	612	2	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	603	2	-	10/39/115/115	-
27	SQD	A	410	-	-	23/47/67/69	0/1/1/1
31	STE	C	519	-	-	5/9/9/17	-
26	LMG	b	622	-	-	27/50/70/70	0/1/1/1
22	CLA	c	513	3	-	9/39/115/115	-
30	BCR	C	514	-	-	8/29/63/63	0/2/2/2
29	DGD	A	413	-	-	28/55/95/95	0/2/2/2
22	CLA	c	505	3	-	13/39/115/115	-
22	CLA	d	404	36	-	1/39/115/115	-
26	LMG	A	409	-	-	16/43/63/70	0/1/1/1
22	CLA	C	507	36	-	6/39/115/115	-
22	CLA	B	613	2	-	15/39/115/115	-
22	CLA	c	510	3	-	12/39/115/115	-
29	DGD	c	517	-	-	14/51/91/95	0/2/2/2
22	CLA	c	512	3	-	20/39/115/115	-
31	STE	t	103	-	-	5/11/11/17	-
22	CLA	C	509	3	-	16/39/115/115	-
31	STE	R	101	-	-	4/9/9/17	-
31	STE	b	620	-	-	6/13/13/17	-
27	SQD	A	412	-	-	19/39/39/69	-
31	STE	a	412	-	-	4/9/9/17	-
22	CLA	b	610	36	-	7/39/115/115	-
25	PL9	D	407	-	-	14/53/73/73	0/1/1/1
31	STE	B	624	-	-	7/13/13/17	-
26	LMG	c	518	-	-	11/31/51/70	0/1/1/1

All (991) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	612	CLA	MG-ND	-12.14	1.81	2.05
22	b	610	CLA	MG-NB	-10.90	1.84	2.05
22	b	615	CLA	MG-ND	-10.89	1.84	2.05
23	d	401	PHO	C1B-C2B	9.91	1.50	1.39
22	B	605	CLA	MG-NA	9.19	2.28	2.06
22	b	606	CLA	MG-NA	9.02	2.27	2.06
22	C	502	CLA	MG-NB	-8.93	1.88	2.05
23	a	404	PHO	C1B-C2B	8.80	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	501	CLA	MG-NB	-8.78	1.88	2.05
22	c	507	CLA	MG-NB	-8.59	1.88	2.05
23	d	401	PHO	C3B-C4B	8.39	1.50	1.41
22	b	615	CLA	MG-NA	8.29	2.26	2.06
23	D	401	PHO	C1B-C2B	8.26	1.48	1.39
23	D	401	PHO	C3B-C4B	7.97	1.49	1.41
34	F	101	HEC	C3D-C2D	7.70	1.53	1.36
22	D	405	CLA	MG-NB	-7.67	1.90	2.05
22	H	101	CLA	MG-NA	7.61	2.24	2.06
22	b	603	CLA	MG-NA	7.51	2.24	2.06
22	d	404	CLA	MG-NA	7.50	2.24	2.06
22	b	613	CLA	MG-NB	-7.12	1.91	2.05
34	v	201	HEC	C3D-C2D	7.11	1.52	1.36
34	f	101	HEC	C3D-C2D	6.99	1.51	1.36
22	d	405	CLA	MG-NA	6.92	2.22	2.06
22	C	506	CLA	MG-ND	-6.85	1.92	2.05
22	c	511	CLA	MG-NA	6.81	2.22	2.06
23	a	404	PHO	C3B-C4B	6.79	1.48	1.41
22	c	507	CLA	MG-NA	6.69	2.22	2.06
22	b	602	CLA	MG-NB	-6.51	1.92	2.05
22	c	506	CLA	MG-ND	-6.47	1.93	2.05
23	A	404	PHO	C1B-C2B	6.46	1.46	1.39
22	b	609	CLA	MG-NC	6.40	2.21	2.06
22	B	610	CLA	MG-NA	6.37	2.21	2.06
22	a	405	CLA	MG-ND	-6.33	1.93	2.05
22	C	501	CLA	MG-NB	-6.32	1.93	2.05
22	D	404	CLA	MG-NA	6.19	2.21	2.06
22	B	615	CLA	MG-NC	6.18	2.20	2.06
22	C	508	CLA	MG-NA	6.17	2.20	2.06
22	B	607	CLA	MG-NA	6.12	2.20	2.06
22	C	511	CLA	MG-NA	6.06	2.20	2.06
22	b	614	CLA	MG-NC	6.01	2.20	2.06
30	b	618	BCR	C30-C25	-5.99	1.46	1.53
34	V	201	HEC	C3D-C2D	5.93	1.49	1.36
22	B	607	CLA	MG-NC	-5.90	1.92	2.06
22	C	501	CLA	MG-NA	5.80	2.20	2.06
23	d	401	PHO	C1D-C2D	5.79	1.45	1.39
22	b	614	CLA	MG-ND	5.79	2.17	2.05
34	V	201	HEC	FE-ND	5.78	2.12	1.94
22	C	508	CLA	MG-ND	5.66	2.17	2.05
22	B	601	CLA	MG-NB	-5.64	1.94	2.05
23	A	404	PHO	C3B-C4B	5.61	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	514	BCR	C1-C6	-5.58	1.46	1.53
22	C	503	CLA	MG-NC	5.50	2.19	2.06
22	A	403	CLA	C4B-NB	5.49	1.45	1.37
25	A	408	PL9	C7-C3	-5.49	1.44	1.51
22	b	615	CLA	MG-NB	5.44	2.16	2.05
22	c	501	CLA	MG-NA	5.44	2.19	2.06
22	d	405	CLA	MG-NC	-5.38	1.93	2.06
22	B	603	CLA	MG-NA	5.37	2.19	2.06
22	c	512	CLA	MG-NC	5.33	2.18	2.06
22	C	510	CLA	MG-NB	5.27	2.16	2.05
22	c	506	CLA	MG-NB	5.24	2.16	2.05
22	b	607	CLA	MG-NB	-5.22	1.95	2.05
26	m	101	LMG	C4-C3	5.20	1.65	1.52
22	c	512	CLA	MG-ND	5.05	2.15	2.05
22	B	606	CLA	MG-NC	-5.02	1.94	2.06
22	D	405	CLA	MG-NC	4.96	2.18	2.06
22	D	405	CLA	MG-ND	-4.94	1.96	2.05
22	c	507	CLA	MG-NC	-4.88	1.94	2.06
34	f	101	HEC	FE-ND	4.88	2.09	1.94
22	B	601	CLA	C1D-ND	4.87	1.44	1.37
22	D	403	CLA	MG-NA	4.84	2.17	2.06
22	C	506	CLA	MG-NB	4.83	2.15	2.05
25	A	408	PL9	C3-C4	-4.81	1.42	1.49
22	b	611	CLA	MG-NA	4.81	2.17	2.06
22	c	509	CLA	MG-NC	-4.78	1.94	2.06
22	b	610	CLA	MG-ND	4.72	2.15	2.05
22	a	405	CLA	C1D-ND	4.66	1.44	1.37
22	b	613	CLA	MG-ND	4.63	2.15	2.05
22	B	605	CLA	MG-NB	4.62	2.14	2.05
25	D	407	PL9	C52-C5	-4.60	1.41	1.50
22	c	509	CLA	MG-ND	4.58	2.14	2.05
22	B	605	CLA	MG-NC	-4.57	1.95	2.06
29	c	515	DGD	O5D-C6D	-4.56	1.35	1.43
22	c	502	CLA	MG-NB	-4.55	1.96	2.05
22	B	606	CLA	MG-NA	4.54	2.17	2.06
22	b	609	CLA	MG-ND	-4.50	1.96	2.05
22	D	405	CLA	C1D-ND	4.49	1.43	1.37
25	A	408	PL9	C7-C8	-4.46	1.43	1.50
22	B	609	CLA	MG-NA	4.44	2.16	2.06
22	b	602	CLA	C1D-ND	4.43	1.43	1.37
25	d	407	PL9	C3-C4	-4.40	1.42	1.49
22	c	506	CLA	C1D-ND	4.37	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	602	CLA	MG-NA	4.35	2.16	2.06
22	a	402	CLA	MG-NA	4.35	2.16	2.06
22	C	509	CLA	MG-NA	4.34	2.16	2.06
30	b	619	BCR	C1-C6	-4.31	1.48	1.53
22	B	613	CLA	C4B-NB	4.31	1.43	1.37
22	b	604	CLA	MG-NC	4.31	2.16	2.06
26	a	414	LMG	C4-C5	4.29	1.62	1.53
29	H	103	DGD	C1E-C2E	4.29	1.65	1.52
26	A	409	LMG	O1-C7	-4.28	1.36	1.43
30	k	101	BCR	C1-C6	-4.27	1.48	1.53
25	d	407	PL9	C53-C6	-4.26	1.42	1.50
29	A	413	DGD	C4D-C5D	4.25	1.62	1.53
30	K	102	BCR	C1-C6	-4.23	1.48	1.53
22	d	403	CLA	C1D-ND	4.23	1.43	1.37
30	K	102	BCR	C30-C25	-4.22	1.48	1.53
30	b	617	BCR	C1-C6	-4.18	1.48	1.53
22	a	403	CLA	MG-NB	4.16	2.14	2.05
22	c	502	CLA	MG-NC	-4.16	1.96	2.06
22	d	405	CLA	MG-NB	-4.14	1.97	2.05
34	F	101	HEC	FE-NC	4.13	2.08	1.95
25	a	409	PL9	C53-C6	-4.12	1.42	1.50
30	H	102	BCR	C30-C25	-4.12	1.48	1.53
22	C	507	CLA	C1B-NB	-4.10	1.32	1.37
23	D	401	PHO	CMD-C2D	-4.10	1.43	1.51
22	c	502	CLA	MG-NA	4.09	2.16	2.06
22	D	403	CLA	C1D-ND	4.08	1.43	1.37
22	c	512	CLA	C4B-NB	4.07	1.43	1.37
22	d	403	CLA	MG-NC	4.06	2.15	2.06
30	t	101	BCR	C30-C25	-4.06	1.48	1.53
22	b	606	CLA	C1D-ND	4.06	1.43	1.37
30	B	618	BCR	C1-C6	-4.03	1.48	1.53
22	b	609	CLA	C1D-ND	4.02	1.43	1.37
22	C	502	CLA	MG-NA	4.01	2.15	2.06
22	c	513	CLA	MG-ND	-4.01	1.97	2.05
22	d	405	CLA	C1D-ND	4.00	1.43	1.37
22	b	605	CLA	MG-ND	4.00	2.13	2.05
26	D	412	LMG	C7-C8	3.99	1.60	1.51
22	c	506	CLA	MG-NA	3.98	2.15	2.06
22	C	504	CLA	C1B-NB	-3.98	1.32	1.37
30	K	101	BCR	C30-C25	-3.96	1.48	1.53
22	c	511	CLA	C4B-NB	3.96	1.43	1.37
30	D	406	BCR	C30-C25	-3.95	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	514	BCR	C1-C6	-3.94	1.48	1.53
22	d	403	CLA	MG-NB	-3.94	1.98	2.05
22	b	601	CLA	MG-NA	3.94	2.15	2.06
22	C	512	CLA	MG-ND	3.93	2.13	2.05
29	A	413	DGD	C3G-C2G	3.91	1.63	1.50
25	D	407	PL9	C11-C9	-3.91	1.43	1.51
22	C	505	CLA	CHC-C1C	3.91	1.46	1.38
22	c	511	CLA	C1B-C2B	3.90	1.52	1.43
22	D	404	CLA	C1D-ND	3.90	1.43	1.37
22	b	614	CLA	MG-NB	-3.89	1.98	2.05
22	B	614	CLA	CMB-C2B	-3.87	1.42	1.50
22	B	611	CLA	MG-NA	3.86	2.15	2.06
22	b	603	CLA	MG-NC	-3.86	1.97	2.06
22	c	508	CLA	MG-NB	3.86	2.13	2.05
26	D	408	LMG	C4-C5	3.86	1.61	1.53
22	c	507	CLA	MG-ND	3.86	2.13	2.05
22	b	612	CLA	MG-ND	-3.86	1.98	2.05
26	B	620	LMG	O8-C28	3.83	1.43	1.30
23	A	404	PHO	C4D-CHA	3.82	1.45	1.39
30	b	618	BCR	C1-C6	-3.82	1.48	1.53
22	C	507	CLA	C1D-ND	3.81	1.42	1.37
26	m	101	LMG	O1-C7	-3.81	1.37	1.43
22	D	404	CLA	MG-ND	3.81	2.13	2.05
26	M	101	LMG	C1-C2	3.80	1.63	1.52
29	C	516	DGD	O5D-C6D	-3.78	1.37	1.43
22	B	615	CLA	MG-ND	3.78	2.13	2.05
22	b	609	CLA	C4B-NB	3.78	1.42	1.37
22	C	513	CLA	C1D-ND	3.77	1.42	1.37
26	d	410	LMG	C4-C5	3.77	1.61	1.53
22	b	612	CLA	MG-NC	3.77	2.15	2.06
22	C	503	CLA	MG-ND	3.77	2.13	2.05
26	c	521	LMG	C3-C2	3.76	1.62	1.52
26	a	414	LMG	O1-C7	3.76	1.50	1.43
23	D	401	PHO	C4D-ND	-3.76	1.32	1.38
22	d	403	CLA	C1B-NB	-3.76	1.32	1.37
22	b	615	CLA	C1D-ND	3.74	1.42	1.37
30	T	101	BCR	C30-C25	-3.73	1.49	1.53
27	A	412	SQD	O48-C23	3.72	1.44	1.33
23	D	401	PHO	CAC-C3C	-3.72	1.45	1.51
26	c	518	LMG	C4-C5	3.72	1.60	1.53
27	A	412	SQD	O47-C7	3.71	1.44	1.34
22	B	613	CLA	MG-NB	-3.71	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	x	101	BCR	C30-C25	-3.70	1.49	1.53
27	L	101	SQD	O48-C23	3.67	1.44	1.33
30	k	102	BCR	C30-C25	-3.65	1.49	1.53
22	c	508	CLA	C1D-ND	3.64	1.42	1.37
27	a	410	SQD	O48-C23	3.64	1.43	1.33
22	C	512	CLA	MG-NB	3.63	2.13	2.05
22	B	601	CLA	C4B-NB	3.63	1.42	1.37
30	I	101	BCR	C1-C6	-3.62	1.49	1.53
29	C	518	DGD	O1G-C1G	-3.61	1.37	1.45
22	c	509	CLA	MG-NB	-3.61	1.98	2.05
27	B	621	SQD	O47-C7	3.61	1.44	1.34
22	B	611	CLA	C1D-ND	3.60	1.42	1.37
30	d	406	BCR	C30-C25	-3.59	1.49	1.53
27	A	410	SQD	O47-C7	3.59	1.44	1.34
28	D	411	LHG	P-O6	3.59	1.73	1.59
22	c	512	CLA	MG-NA	-3.58	1.97	2.06
22	b	614	CLA	C1B-NB	-3.57	1.33	1.37
34	v	201	HEC	FE-NB	3.56	2.05	1.94
22	C	501	CLA	C1D-ND	3.55	1.42	1.37
30	a	406	BCR	C30-C25	-3.55	1.49	1.53
22	c	512	CLA	CHC-C1C	3.55	1.45	1.38
25	d	407	PL9	C16-C14	-3.54	1.44	1.51
25	D	407	PL9	C6-C1	-3.53	1.42	1.48
30	k	103	BCR	C30-C25	-3.53	1.49	1.53
27	D	409	SQD	O48-C23	3.53	1.43	1.33
22	c	510	CLA	C1D-ND	3.52	1.42	1.37
22	B	612	CLA	C4B-NB	3.52	1.42	1.37
22	b	616	CLA	MG-ND	-3.52	1.98	2.05
22	C	510	CLA	MG-NA	3.51	2.14	2.06
34	F	101	HEC	FE-ND	3.51	2.05	1.94
22	C	506	CLA	MG-NC	3.50	2.14	2.06
22	b	611	CLA	C1B-C2B	3.49	1.51	1.43
29	c	515	DGD	O2G-C2G	-3.48	1.38	1.46
27	t	102	SQD	O48-C23	3.48	1.43	1.33
22	b	612	CLA	C1D-ND	3.48	1.42	1.37
28	d	409	LHG	P-O6	3.46	1.73	1.59
22	b	604	CLA	MG-NA	-3.46	1.98	2.06
22	C	506	CLA	C4B-NB	3.45	1.42	1.37
22	b	602	CLA	C4B-NB	3.45	1.42	1.37
22	B	610	CLA	MG-NB	-3.45	1.99	2.05
28	D	411	LHG	O3-C3	-3.44	1.31	1.44
22	B	610	CLA	CMD-C2D	-3.44	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	516	DGD	O1G-C1A	3.44	1.43	1.33
29	H	103	DGD	C4E-C5E	3.44	1.60	1.53
22	c	503	CLA	MG-NA	3.43	2.14	2.06
29	C	518	DGD	O3G-C3G	-3.43	1.37	1.43
27	t	102	SQD	O47-C7	3.43	1.44	1.34
22	A	403	CLA	C1B-C2B	3.43	1.51	1.43
27	L	101	SQD	O47-C7	3.42	1.43	1.34
22	C	504	CLA	MG-ND	-3.42	1.99	2.05
22	c	502	CLA	C1D-ND	3.42	1.42	1.37
22	c	511	CLA	C1D-ND	3.42	1.42	1.37
26	D	412	LMG	C9-C8	3.42	1.61	1.50
22	c	501	CLA	CMC-C2C	-3.41	1.43	1.50
22	B	610	CLA	MG-NC	-3.41	1.98	2.06
22	B	601	CLA	C1B-C2B	3.40	1.51	1.43
22	B	609	CLA	MG-NC	-3.39	1.98	2.06
27	A	410	SQD	O48-C23	3.39	1.43	1.33
22	a	402	CLA	C1B-C2B	3.38	1.51	1.43
27	B	621	SQD	O48-C23	3.37	1.43	1.33
22	B	615	CLA	C1D-ND	3.34	1.42	1.37
26	a	414	LMG	O8-C9	-3.34	1.37	1.45
22	b	605	CLA	CMC-C2C	-3.34	1.43	1.50
22	B	609	CLA	C1D-ND	3.33	1.42	1.37
22	a	402	CLA	C1D-ND	3.32	1.42	1.37
22	A	402	CLA	MG-NC	-3.32	1.98	2.06
23	A	404	PHO	C4D-ND	-3.31	1.33	1.38
28	A	411	LHG	C24-C23	3.30	1.60	1.50
22	b	601	CLA	C1B-C2B	3.28	1.50	1.43
34	f	101	HEC	FE-NA	3.28	2.06	1.95
22	A	403	CLA	C1D-ND	3.28	1.42	1.37
22	b	615	CLA	C4B-NB	3.28	1.42	1.37
29	A	413	DGD	O5D-C1E	3.27	1.45	1.40
28	L	102	LHG	O7-C5	-3.27	1.38	1.46
22	B	608	CLA	CMD-C2D	-3.27	1.44	1.50
30	k	103	BCR	C1-C6	-3.27	1.49	1.53
28	D	413	LHG	O7-C5	-3.27	1.38	1.46
22	b	604	CLA	C1B-NB	-3.26	1.33	1.37
30	K	101	BCR	C1-C6	-3.26	1.49	1.53
22	B	609	CLA	MG-NB	3.25	2.12	2.05
26	M	101	LMG	O7-C8	-3.25	1.39	1.46
26	d	410	LMG	O1-C7	-3.24	1.38	1.43
22	C	511	CLA	C1D-ND	3.23	1.42	1.37
22	c	508	CLA	MG-NC	3.23	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	520	LMG	C3-C2	3.23	1.60	1.52
34	V	201	HEC	FE-NA	3.23	2.05	1.95
22	B	611	CLA	C1B-C2B	3.22	1.50	1.43
22	a	405	CLA	C1B-C2B	3.22	1.50	1.43
22	B	603	CLA	C1D-ND	3.22	1.42	1.37
22	A	402	CLA	C4B-NB	3.22	1.42	1.37
26	Y	101	LMG	C4-C5	3.22	1.59	1.53
22	c	504	CLA	C4B-NB	3.21	1.42	1.37
30	B	616	BCR	C30-C25	-3.21	1.49	1.53
26	c	518	LMG	C1-C2	3.21	1.61	1.52
22	b	603	CLA	CMC-C2C	-3.21	1.44	1.50
30	B	616	BCR	C1-C6	-3.20	1.49	1.53
22	A	403	CLA	MG-NA	3.20	2.13	2.06
30	k	101	BCR	C30-C25	-3.20	1.49	1.53
22	c	501	CLA	C4B-NB	3.20	1.42	1.37
22	b	602	CLA	CMD-C2D	-3.19	1.44	1.50
22	A	405	CLA	C1D-ND	3.19	1.42	1.37
29	H	103	DGD	C6D-C5D	3.19	1.61	1.51
22	d	404	CLA	C1B-C2B	3.18	1.50	1.43
22	b	610	CLA	MG-NC	-3.18	1.98	2.06
26	A	409	LMG	C4-C3	3.18	1.60	1.52
22	C	505	CLA	C1B-NB	-3.16	1.33	1.37
22	A	402	CLA	C1B-C2B	3.16	1.50	1.43
22	b	603	CLA	CMD-C2D	-3.15	1.44	1.50
29	c	517	DGD	O2E-C2E	-3.15	1.35	1.43
22	B	611	CLA	C4B-NB	3.15	1.42	1.37
22	B	613	CLA	MG-NA	3.15	2.13	2.06
22	b	601	CLA	C4B-NB	3.14	1.42	1.37
22	B	612	CLA	CMD-C2D	-3.14	1.44	1.50
22	c	504	CLA	MG-NB	-3.14	1.99	2.05
22	c	513	CLA	C4B-NB	3.13	1.42	1.37
22	H	101	CLA	C1B-C2B	3.13	1.50	1.43
22	c	513	CLA	C1B-C2B	3.13	1.50	1.43
22	B	612	CLA	C1D-ND	3.12	1.42	1.37
23	a	404	PHO	C1D-C2D	3.12	1.43	1.39
26	c	521	LMG	C1-C2	3.11	1.61	1.52
22	C	507	CLA	MG-ND	-3.11	1.99	2.05
22	D	405	CLA	MG-NA	-3.11	1.98	2.06
25	d	407	PL9	C21-C19	-3.10	1.44	1.51
22	c	509	CLA	C1B-C2B	3.09	1.50	1.43
28	a	411	LHG	P-O6	3.09	1.71	1.59
27	f	102	SQD	O47-C7	3.08	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	405	CLA	CMD-C2D	-3.08	1.44	1.50
26	b	622	LMG	O6-C1	3.08	1.49	1.41
22	B	608	CLA	MG-NA	3.07	2.13	2.06
29	C	517	DGD	C6D-C5D	3.07	1.60	1.51
29	A	413	DGD	C1E-C2E	3.06	1.61	1.52
25	D	407	PL9	C26-C24	-3.06	1.45	1.51
22	H	101	CLA	C4B-NB	3.06	1.41	1.37
22	b	614	CLA	C1D-ND	3.05	1.41	1.37
22	c	501	CLA	CMB-C2B	-3.05	1.44	1.50
29	C	516	DGD	C3G-C2G	3.05	1.60	1.50
22	b	608	CLA	CHC-C1C	3.05	1.44	1.38
23	d	401	PHO	CAC-C3C	-3.05	1.46	1.51
29	c	516	DGD	O2E-C2E	-3.05	1.35	1.43
22	a	403	CLA	C1B-C2B	3.03	1.50	1.43
29	C	517	DGD	C1E-C2E	3.03	1.61	1.52
22	b	606	CLA	C4B-NB	3.03	1.41	1.37
22	A	402	CLA	C1D-ND	3.03	1.41	1.37
26	M	101	LMG	C7-C8	3.02	1.60	1.50
22	c	501	CLA	C1D-ND	3.01	1.41	1.37
28	b	623	LHG	O7-C5	-3.00	1.39	1.46
30	C	515	BCR	C1-C6	-3.00	1.49	1.53
30	t	101	BCR	C1-C6	-2.99	1.50	1.53
28	l	101	LHG	O7-C5	-2.99	1.39	1.46
22	d	403	CLA	CMB-C2B	-2.99	1.44	1.50
23	d	401	PHO	CMC-C2C	-2.99	1.46	1.50
22	b	607	CLA	C1D-ND	2.98	1.41	1.37
22	B	614	CLA	MG-ND	2.98	2.11	2.05
25	D	407	PL9	C53-C6	-2.98	1.44	1.50
22	b	609	CLA	CMB-C2B	-2.98	1.44	1.50
23	d	401	PHO	C4D-CHA	2.97	1.44	1.39
27	a	410	SQD	O47-C7	2.97	1.42	1.34
28	D	410	LHG	O7-C5	-2.97	1.39	1.46
22	c	503	CLA	C1D-ND	2.97	1.41	1.37
23	A	404	PHO	CMD-C2D	-2.96	1.45	1.51
29	c	517	DGD	C3G-C2G	2.96	1.60	1.50
22	c	512	CLA	C1D-ND	2.95	1.41	1.37
27	f	102	SQD	O48-C23	2.95	1.42	1.33
22	B	609	CLA	CMB-C2B	-2.95	1.44	1.50
22	c	501	CLA	C1B-C2B	2.95	1.50	1.43
22	a	403	CLA	C1D-ND	2.95	1.41	1.37
22	A	405	CLA	MG-NB	-2.95	1.99	2.05
28	A	411	LHG	P-O6	2.94	1.70	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D	406	BCR	C1-C6	-2.94	1.50	1.53
30	B	618	BCR	C30-C25	-2.94	1.50	1.53
22	b	614	CLA	CHC-C1C	2.94	1.44	1.38
23	a	404	PHO	C3D-C4D	2.93	1.45	1.41
22	b	611	CLA	CMD-C2D	-2.93	1.44	1.50
22	B	601	CLA	MG-NA	2.92	2.13	2.06
22	c	507	CLA	C1B-C2B	2.92	1.50	1.43
22	B	606	CLA	C1B-C2B	2.92	1.50	1.43
22	B	601	CLA	CMB-C2B	-2.91	1.44	1.50
22	C	501	CLA	CMD-C2D	-2.91	1.44	1.50
22	C	509	CLA	CMD-C2D	-2.91	1.44	1.50
22	C	510	CLA	C4B-NB	2.91	1.41	1.37
22	B	608	CLA	C1B-C2B	2.90	1.49	1.43
22	A	403	CLA	CMB-C2B	-2.90	1.44	1.50
22	c	505	CLA	C4B-NB	2.90	1.41	1.37
25	A	408	PL9	C6-C1	-2.89	1.43	1.48
29	H	103	DGD	O5D-C1E	2.89	1.45	1.40
22	H	101	CLA	C1D-ND	2.89	1.41	1.37
22	c	502	CLA	CMD-C2D	-2.89	1.44	1.50
29	A	413	DGD	C4E-C5E	2.88	1.59	1.53
30	I	101	BCR	C33-C5	-2.88	1.46	1.50
22	H	101	CLA	MG-ND	-2.88	2.00	2.05
26	d	410	LMG	O7-C8	-2.88	1.39	1.46
22	B	604	CLA	C1B-C2B	2.87	1.49	1.43
22	B	615	CLA	CMB-C2B	-2.87	1.44	1.50
22	b	604	CLA	C4B-NB	2.87	1.41	1.37
22	d	404	CLA	CMB-C2B	-2.87	1.44	1.50
22	B	612	CLA	C1B-C2B	2.87	1.49	1.43
22	B	614	CLA	C4B-NB	2.87	1.41	1.37
22	C	511	CLA	C1B-C2B	2.87	1.49	1.43
22	C	501	CLA	MG-ND	2.86	2.11	2.05
29	c	515	DGD	C3D-C2D	2.86	1.59	1.52
22	b	601	CLA	C1D-ND	2.86	1.41	1.37
22	C	508	CLA	C1B-C2B	2.86	1.49	1.43
22	C	505	CLA	MG-NB	2.86	2.11	2.05
22	c	513	CLA	C1D-ND	2.86	1.41	1.37
22	c	506	CLA	C1B-NB	-2.85	1.34	1.37
22	B	615	CLA	CMD-C2D	-2.85	1.44	1.50
22	B	610	CLA	MG-ND	2.85	2.11	2.05
26	A	409	LMG	O8-C9	-2.84	1.38	1.45
22	C	512	CLA	MG-NA	2.84	2.13	2.06
22	C	513	CLA	CMB-C2B	-2.84	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	503	CLA	CMB-C2B	-2.84	1.45	1.50
22	b	615	CLA	MG-NC	-2.83	1.99	2.06
22	B	602	CLA	C1B-C2B	2.83	1.49	1.43
29	C	516	DGD	C4E-C3E	2.83	1.59	1.52
22	C	503	CLA	C1B-C2B	2.83	1.49	1.43
22	c	504	CLA	CMD-C2D	-2.83	1.45	1.50
22	b	613	CLA	CMD-C2D	-2.82	1.45	1.50
29	C	518	DGD	O2G-C2G	-2.82	1.40	1.46
30	b	619	BCR	C30-C25	-2.82	1.50	1.53
22	d	404	CLA	C4B-NB	2.82	1.41	1.37
22	H	101	CLA	CHC-C1C	2.82	1.44	1.38
26	b	622	LMG	O8-C28	2.81	1.41	1.33
22	C	504	CLA	C1D-ND	2.81	1.41	1.37
22	C	513	CLA	C4B-NB	2.81	1.41	1.37
22	b	616	CLA	CMD-C2D	-2.81	1.45	1.50
22	D	405	CLA	C1B-C2B	2.81	1.49	1.43
22	C	503	CLA	C1D-ND	2.81	1.41	1.37
22	b	616	CLA	C1D-ND	2.80	1.41	1.37
22	C	509	CLA	MG-NC	-2.80	1.99	2.06
30	d	406	BCR	C1-C6	-2.80	1.50	1.53
22	c	513	CLA	CMD-C2D	-2.80	1.45	1.50
29	c	516	DGD	C3D-C2D	2.80	1.59	1.52
22	c	511	CLA	MG-ND	-2.79	2.00	2.05
28	a	411	LHG	O8-C23	2.79	1.41	1.33
26	a	414	LMG	C3-C2	2.79	1.59	1.52
23	a	404	PHO	C4D-ND	-2.78	1.34	1.38
22	C	506	CLA	C1D-ND	2.78	1.41	1.37
29	c	517	DGD	C4D-C5D	2.77	1.58	1.53
22	b	613	CLA	C1D-ND	2.77	1.41	1.37
22	H	101	CLA	CMB-C2B	-2.77	1.45	1.50
22	c	504	CLA	C1B-C2B	2.77	1.49	1.43
22	B	615	CLA	MG-NB	-2.77	2.00	2.05
34	F	101	HEC	FE-NB	2.77	2.03	1.94
22	c	502	CLA	CMC-C2C	-2.76	1.45	1.50
22	C	506	CLA	CHC-C1C	2.76	1.44	1.38
22	B	605	CLA	C1B-C2B	2.76	1.49	1.43
22	B	602	CLA	C1D-ND	2.75	1.41	1.37
26	a	414	LMG	O7-C10	2.75	1.42	1.34
22	B	609	CLA	C3B-C4B	2.75	1.50	1.42
22	B	614	CLA	C1D-ND	2.75	1.41	1.37
28	D	410	LHG	O8-C6	-2.75	1.39	1.45
22	a	403	CLA	CHC-C1C	2.75	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	413	DGD	O1G-C1A	2.75	1.41	1.33
22	B	606	CLA	C1D-ND	2.75	1.41	1.37
22	b	610	CLA	C1B-C2B	2.75	1.49	1.43
22	A	405	CLA	C1B-C2B	2.74	1.49	1.43
26	Y	101	LMG	O7-C8	-2.74	1.40	1.46
22	B	614	CLA	MG-NB	-2.74	2.00	2.05
22	c	509	CLA	C1D-ND	2.73	1.41	1.37
23	A	404	PHO	C3B-C2B	-2.73	1.36	1.40
28	L	102	LHG	P-O6	2.73	1.70	1.59
22	c	508	CLA	CHC-C1C	2.73	1.43	1.38
22	B	603	CLA	C3B-C4B	2.73	1.50	1.42
22	B	614	CLA	C1B-C2B	2.73	1.49	1.43
26	c	518	LMG	O1-C1	2.73	1.44	1.40
22	b	605	CLA	C1B-C2B	2.72	1.49	1.43
22	C	506	CLA	C1B-C2B	2.72	1.49	1.43
22	b	610	CLA	CHC-C4B	-2.72	1.33	1.39
22	b	612	CLA	CMB-C2B	-2.72	1.45	1.50
22	b	602	CLA	C3B-C4B	2.72	1.50	1.42
22	C	512	CLA	C1B-C2B	2.72	1.49	1.43
22	b	602	CLA	C1B-C2B	2.71	1.49	1.43
22	A	403	CLA	CMD-C2D	-2.71	1.45	1.50
22	c	506	CLA	CMB-C2B	-2.71	1.45	1.50
26	a	414	LMG	C1-C2	2.71	1.60	1.52
22	b	615	CLA	C3B-C4B	2.70	1.50	1.42
25	D	407	PL9	C45-C44	-2.70	1.44	1.50
22	b	603	CLA	CMB-C2B	-2.70	1.45	1.50
22	B	611	CLA	C3B-C4B	2.70	1.50	1.42
22	c	512	CLA	C3B-C4B	2.69	1.50	1.42
22	D	405	CLA	C4B-NB	2.69	1.41	1.37
29	H	103	DGD	O2D-C2D	-2.69	1.36	1.43
26	Y	101	LMG	C6-C5	2.69	1.60	1.51
26	c	520	LMG	O1-C1	2.68	1.44	1.40
25	d	407	PL9	C7-C8	-2.68	1.46	1.50
22	B	610	CLA	C1B-NB	-2.67	1.34	1.37
22	C	504	CLA	C4B-NB	2.67	1.41	1.37
22	b	603	CLA	C3B-C4B	2.66	1.50	1.42
22	C	501	CLA	CHC-C1C	2.66	1.43	1.38
22	a	403	CLA	CMD-C2D	-2.66	1.45	1.50
22	d	405	CLA	CMD-C2D	-2.66	1.45	1.50
29	C	517	DGD	O3G-C3G	-2.66	1.39	1.43
29	c	517	DGD	O4E-C4E	-2.66	1.36	1.43
29	C	516	DGD	O2G-C2G	-2.66	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	404	CLA	C1B-C2B	2.65	1.49	1.43
22	B	607	CLA	C1B-NB	-2.65	1.34	1.37
22	b	601	CLA	O2A-CGA	2.65	1.41	1.33
22	a	403	CLA	C4B-NB	2.64	1.41	1.37
22	B	614	CLA	CHC-C4B	-2.64	1.33	1.39
26	Y	101	LMG	C3-C2	2.64	1.59	1.52
22	b	612	CLA	C3B-C4B	2.64	1.50	1.42
22	d	403	CLA	C3D-C4D	2.64	1.50	1.44
22	B	610	CLA	C1B-C2B	2.64	1.49	1.43
22	B	608	CLA	C1D-ND	2.64	1.41	1.37
22	A	405	CLA	CMC-C2C	-2.64	1.45	1.50
26	Y	101	LMG	O8-C9	-2.64	1.39	1.45
22	A	405	CLA	CMD-C2D	-2.64	1.45	1.50
22	C	513	CLA	C3B-C4B	2.63	1.50	1.42
22	A	403	CLA	MG-ND	-2.63	2.00	2.05
22	b	611	CLA	C4B-NB	2.62	1.41	1.37
29	C	517	DGD	C4D-C3D	2.62	1.59	1.52
29	c	516	DGD	C3E-C2E	2.62	1.59	1.52
22	B	609	CLA	C1B-C2B	2.62	1.49	1.43
22	c	510	CLA	CMB-C2B	-2.61	1.45	1.50
23	D	401	PHO	CMB-C2B	-2.61	1.46	1.51
22	C	510	CLA	C1B-C2B	2.61	1.49	1.43
30	a	406	BCR	C38-C26	-2.60	1.46	1.50
29	C	516	DGD	C1D-C2D	2.60	1.60	1.52
22	B	615	CLA	CMC-C2C	-2.60	1.45	1.50
22	B	611	CLA	MG-ND	-2.60	2.00	2.05
22	a	402	CLA	MG-NB	2.60	2.10	2.05
22	b	616	CLA	C1B-C2B	2.60	1.49	1.43
22	a	402	CLA	C3D-C4D	2.60	1.50	1.44
23	A	404	PHO	CMC-C2C	-2.60	1.46	1.50
22	b	613	CLA	MG-NC	2.60	2.12	2.06
22	b	615	CLA	CMB-C2B	-2.59	1.45	1.50
22	b	602	CLA	MG-ND	2.59	2.10	2.05
30	I	101	BCR	C34-C9	-2.59	1.45	1.50
22	B	605	CLA	CHC-C1C	2.59	1.43	1.38
23	d	401	PHO	CBD-CGD	-2.59	1.49	1.52
22	C	511	CLA	C4B-NB	2.59	1.41	1.37
29	c	517	DGD	C2A-C1A	-2.58	1.43	1.50
25	d	407	PL9	C10-C9	-2.58	1.44	1.50
22	b	615	CLA	C1B-C2B	2.57	1.49	1.43
22	c	510	CLA	C1B-NB	-2.57	1.34	1.37
22	c	505	CLA	MG-NC	-2.57	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	511	CLA	CMB-C2B	-2.57	1.45	1.50
22	d	403	CLA	C1B-C2B	2.57	1.49	1.43
22	B	608	CLA	C4B-NB	2.57	1.41	1.37
29	C	518	DGD	O2D-C2D	-2.57	1.36	1.43
22	B	606	CLA	MG-NB	-2.56	2.00	2.05
22	c	513	CLA	CHC-C1C	2.56	1.43	1.38
22	b	607	CLA	C1B-C2B	2.56	1.49	1.43
22	D	404	CLA	CHC-C1C	2.56	1.43	1.38
26	c	518	LMG	O2-C2	-2.55	1.36	1.43
26	b	622	LMG	C9-C8	2.55	1.58	1.50
22	b	612	CLA	C4B-NB	2.55	1.41	1.37
26	B	620	LMG	O7-C10	2.55	1.39	1.30
22	c	513	CLA	C3B-C4B	2.55	1.50	1.42
22	C	506	CLA	C3B-C4B	2.55	1.50	1.42
22	B	601	CLA	C3B-C4B	2.55	1.50	1.42
30	B	617	BCR	C30-C25	-2.54	1.50	1.53
22	c	503	CLA	C1B-C2B	2.54	1.49	1.43
25	d	407	PL9	C40-C39	-2.54	1.44	1.50
22	C	510	CLA	C1B-NB	-2.54	1.34	1.37
22	D	403	CLA	C1B-C2B	2.54	1.49	1.43
29	H	103	DGD	O6E-C1E	2.53	1.48	1.41
29	C	518	DGD	C2A-C1A	-2.53	1.43	1.50
22	C	511	CLA	C3B-C4B	2.53	1.50	1.42
22	C	503	CLA	C4B-NB	2.53	1.41	1.37
22	c	512	CLA	C1B-C2B	2.52	1.49	1.43
28	l	101	LHG	P-O6	2.52	1.69	1.59
22	b	616	CLA	CMC-C2C	-2.52	1.45	1.50
22	c	511	CLA	C3B-C4B	2.52	1.50	1.42
22	b	605	CLA	C1D-ND	2.52	1.41	1.37
30	x	101	BCR	C1-C6	-2.51	1.50	1.53
22	c	504	CLA	C1D-ND	2.51	1.41	1.37
22	b	615	CLA	CMD-C2D	-2.51	1.45	1.50
26	D	412	LMG	O8-C28	2.51	1.40	1.33
30	k	102	BCR	C1-C6	-2.50	1.50	1.53
23	a	404	PHO	CMB-C2B	-2.50	1.46	1.51
28	D	413	LHG	O8-C23	2.50	1.40	1.33
28	d	409	LHG	C6-C5	2.50	1.58	1.50
22	B	614	CLA	CAB-C3B	-2.50	1.40	1.47
29	A	413	DGD	O5D-C6D	-2.50	1.39	1.43
22	a	402	CLA	CMB-C2B	-2.50	1.45	1.50
22	c	507	CLA	C1D-ND	2.50	1.41	1.37
28	b	623	LHG	C8-C7	-2.50	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	507	CLA	C3D-C4D	2.50	1.49	1.44
34	v	201	HEC	CMD-C2D	2.49	1.55	1.50
23	D	401	PHO	C3B-C2B	-2.49	1.37	1.40
22	B	605	CLA	CMA-C3A	-2.49	1.47	1.53
22	c	503	CLA	CMC-C2C	-2.49	1.45	1.50
22	c	511	CLA	CHC-C1C	2.49	1.43	1.38
22	C	512	CLA	CHC-C1C	2.49	1.43	1.38
22	C	502	CLA	C1B-C2B	2.49	1.49	1.43
22	c	505	CLA	C3B-C4B	2.48	1.50	1.42
22	b	607	CLA	C1B-NB	-2.48	1.34	1.37
22	b	606	CLA	CHC-C1C	2.48	1.43	1.38
23	a	404	PHO	C4D-CHA	2.48	1.43	1.39
30	b	617	BCR	C30-C25	-2.48	1.50	1.53
29	C	517	DGD	C4E-C5E	2.48	1.58	1.53
22	C	512	CLA	CMD-C2D	-2.48	1.45	1.50
22	C	505	CLA	C4B-NB	2.48	1.41	1.37
22	C	508	CLA	MG-NB	-2.48	2.00	2.05
28	d	409	LHG	O8-C6	2.47	1.50	1.45
29	h	101	DGD	O5D-C6D	-2.47	1.39	1.43
22	b	611	CLA	MG-NB	2.47	2.10	2.05
22	a	405	CLA	C1B-NB	-2.47	1.34	1.37
23	A	404	PHO	C1C-NC	-2.47	1.30	1.37
22	C	509	CLA	MG-ND	-2.47	2.00	2.05
22	D	405	CLA	CMC-C2C	-2.47	1.45	1.50
30	t	101	BCR	C27-C26	-2.46	1.46	1.51
29	C	516	DGD	O1A-C1A	2.46	1.29	1.22
22	c	513	CLA	CMB-C2B	-2.46	1.45	1.50
22	c	508	CLA	C3B-C4B	2.46	1.49	1.42
27	A	410	SQD	O2-C2	-2.46	1.36	1.43
22	C	509	CLA	CMB-C2B	-2.45	1.45	1.50
22	d	405	CLA	C1B-C2B	2.45	1.48	1.43
30	T	101	BCR	C38-C26	-2.45	1.47	1.50
23	d	401	PHO	CMD-C2D	-2.45	1.46	1.51
23	a	404	PHO	CMC-C2C	-2.45	1.46	1.50
34	v	201	HEC	FE-NA	2.45	2.03	1.95
30	I	101	BCR	C38-C26	-2.44	1.47	1.50
22	c	503	CLA	MG-NB	2.44	2.10	2.05
22	C	504	CLA	MG-NB	-2.44	2.01	2.05
22	C	512	CLA	CMC-C2C	-2.43	1.45	1.50
22	C	501	CLA	CAC-C3C	-2.43	1.44	1.51
27	a	410	SQD	O3-C3	-2.42	1.37	1.43
22	b	601	CLA	CMB-C2B	-2.42	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	401	PHO	C3D-C4D	2.42	1.44	1.41
22	c	512	CLA	C3D-C4D	2.42	1.49	1.44
22	b	607	CLA	CMB-C2B	-2.42	1.45	1.50
22	d	403	CLA	CHC-C1C	2.42	1.43	1.38
22	b	612	CLA	CMD-C2D	-2.41	1.45	1.50
22	C	510	CLA	CMD-C2D	-2.41	1.45	1.50
29	c	516	DGD	O3D-C3D	-2.41	1.37	1.43
29	c	515	DGD	O3G-C1D	-2.41	1.36	1.40
23	d	401	PHO	C4D-ND	-2.41	1.34	1.38
22	b	605	CLA	C1D-C2D	2.41	1.50	1.45
22	c	504	CLA	CAC-C3C	-2.41	1.44	1.51
29	C	517	DGD	C1G-C2G	2.40	1.58	1.50
29	c	517	DGD	O2G-C1B	2.40	1.41	1.34
22	b	606	CLA	C1B-C2B	2.40	1.48	1.43
22	b	614	CLA	C3B-C4B	2.40	1.49	1.42
22	C	512	CLA	C3B-C4B	2.40	1.49	1.42
22	C	503	CLA	CHC-C1C	2.40	1.43	1.38
22	B	614	CLA	O2A-CGA	2.40	1.40	1.33
25	D	407	PL9	C26-C27	2.40	1.61	1.53
22	b	612	CLA	CMC-C2C	-2.40	1.45	1.50
22	B	604	CLA	C5-C3	-2.40	1.46	1.51
22	D	403	CLA	MG-NC	-2.40	2.00	2.06
22	C	509	CLA	C1D-ND	2.40	1.41	1.37
22	C	510	CLA	C3C-C2C	2.39	1.41	1.36
29	A	413	DGD	O1G-C1G	-2.39	1.39	1.45
22	D	405	CLA	CMB-C2B	-2.39	1.45	1.50
22	C	511	CLA	MG-NC	2.39	2.11	2.06
22	b	604	CLA	C1B-C2B	2.39	1.48	1.43
29	c	517	DGD	O2G-C2G	-2.39	1.41	1.46
22	B	610	CLA	CHC-C4B	-2.39	1.34	1.39
22	C	510	CLA	CHC-C1C	2.38	1.43	1.38
29	h	101	DGD	C4E-C3E	2.37	1.58	1.52
29	c	516	DGD	C4E-C5E	2.37	1.58	1.53
22	C	511	CLA	MG-NB	-2.37	2.01	2.05
34	f	101	HEC	CMC-C2C	2.36	1.55	1.50
29	c	515	DGD	C1E-C2E	2.36	1.59	1.52
22	b	607	CLA	CHD-C1D	-2.36	1.33	1.38
22	B	604	CLA	CMD-C2D	-2.36	1.45	1.50
22	b	607	CLA	CHC-C4B	-2.36	1.34	1.39
22	B	605	CLA	C3B-C4B	2.36	1.49	1.42
22	H	101	CLA	C3B-C4B	2.36	1.49	1.42
22	a	403	CLA	C3B-C4B	2.36	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	501	CLA	CMC-C2C	-2.36	1.45	1.50
22	b	602	CLA	CMB-C2B	-2.36	1.45	1.50
22	b	606	CLA	C3B-C4B	2.35	1.49	1.42
23	d	401	PHO	CMB-C2B	-2.35	1.46	1.51
22	D	403	CLA	C4B-NB	2.35	1.40	1.37
22	b	613	CLA	C1B-C2B	2.35	1.48	1.43
22	C	503	CLA	C3D-C4D	2.35	1.49	1.44
22	D	405	CLA	C1B-NB	-2.35	1.34	1.37
22	c	505	CLA	CHC-C1C	2.35	1.43	1.38
22	B	606	CLA	CMC-C2C	-2.34	1.46	1.50
22	C	505	CLA	CMB-C2B	-2.34	1.46	1.50
22	b	607	CLA	C4B-NB	2.34	1.40	1.37
22	B	612	CLA	CMC-C2C	-2.34	1.46	1.50
25	D	407	PL9	C21-C19	-2.34	1.46	1.51
22	b	613	CLA	CAA-C2A	-2.34	1.49	1.54
22	B	606	CLA	C3B-C4B	2.34	1.49	1.42
22	a	402	CLA	C1D-C2D	2.34	1.50	1.45
26	b	622	LMG	C3-C2	2.34	1.58	1.52
27	D	409	SQD	O4-C4	-2.33	1.37	1.43
22	c	507	CLA	CHC-C4B	-2.33	1.34	1.39
22	b	609	CLA	CHC-C1C	2.33	1.43	1.38
30	B	616	BCR	C33-C5	-2.33	1.47	1.50
22	C	508	CLA	C4B-NB	2.33	1.40	1.37
22	b	605	CLA	CMD-C2D	-2.33	1.46	1.50
22	a	402	CLA	CMC-C2C	-2.33	1.46	1.50
26	c	518	LMG	C7-C8	2.33	1.58	1.50
22	b	606	CLA	CMD-C2D	-2.32	1.46	1.50
22	B	605	CLA	C1D-ND	2.32	1.40	1.37
27	f	102	SQD	O3-C3	-2.32	1.37	1.43
22	b	606	CLA	O2D-CED	-2.32	1.40	1.45
25	d	407	PL9	C26-C24	-2.31	1.46	1.51
30	C	515	BCR	C30-C25	-2.31	1.50	1.53
30	C	514	BCR	C33-C5	-2.31	1.47	1.50
22	A	405	CLA	C4B-NB	2.31	1.40	1.37
22	B	604	CLA	C1B-NB	-2.31	1.34	1.37
26	c	521	LMG	C4-C5	2.31	1.57	1.53
22	b	611	CLA	MG-NC	-2.31	2.00	2.06
22	b	614	CLA	C1B-C2B	2.31	1.48	1.43
26	c	518	LMG	C6-C5	2.31	1.59	1.51
23	A	404	PHO	O2D-CGD	2.31	1.38	1.33
22	b	608	CLA	MG-NB	2.30	2.10	2.05
22	c	505	CLA	C1B-C2B	2.30	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	605	CLA	C4B-NB	2.30	1.40	1.37
22	C	509	CLA	C3B-C4B	2.30	1.49	1.42
22	d	403	CLA	C4B-NB	2.30	1.40	1.37
26	b	622	LMG	C4-C3	2.30	1.58	1.52
26	Y	101	LMG	C1-C2	2.30	1.59	1.52
22	a	403	CLA	CMB-C2B	-2.30	1.46	1.50
27	t	102	SQD	C24-C23	2.30	1.57	1.50
22	b	607	CLA	CMD-C2D	-2.30	1.46	1.50
30	c	514	BCR	C38-C26	-2.29	1.47	1.50
22	C	504	CLA	CMB-C2B	-2.29	1.46	1.50
22	C	508	CLA	C3B-C4B	2.29	1.49	1.42
22	b	608	CLA	C3B-C4B	2.29	1.49	1.42
22	b	604	CLA	C1D-ND	2.29	1.40	1.37
22	C	502	CLA	C1D-ND	2.29	1.40	1.37
22	B	603	CLA	MG-NB	2.29	2.10	2.05
22	b	611	CLA	CHC-C4B	-2.29	1.34	1.39
22	B	613	CLA	C1B-C2B	2.29	1.48	1.43
23	a	404	PHO	C1C-NC	-2.28	1.30	1.37
22	b	605	CLA	C1B-NB	-2.28	1.34	1.37
28	a	411	LHG	C3-C2	2.28	1.58	1.51
22	d	404	CLA	CHB-C1B	2.28	1.44	1.39
22	B	602	CLA	CHC-C4B	-2.28	1.34	1.39
26	m	101	LMG	C1-C2	2.28	1.59	1.52
22	B	612	CLA	C4-C3	-2.28	1.45	1.50
30	k	102	BCR	C38-C26	-2.28	1.47	1.50
29	h	101	DGD	C4E-C5E	2.28	1.57	1.53
22	c	508	CLA	C1B-NB	-2.28	1.34	1.37
29	c	516	DGD	C1E-C2E	2.28	1.59	1.52
30	c	514	BCR	C30-C25	-2.28	1.50	1.53
22	b	607	CLA	CMC-C2C	-2.27	1.46	1.50
25	D	407	PL9	C16-C17	2.27	1.61	1.53
22	B	611	CLA	CMD-C2D	-2.27	1.46	1.50
31	B	619	STE	C2-C1	2.27	1.55	1.50
22	C	505	CLA	CMC-C2C	-2.27	1.46	1.50
22	d	405	CLA	CAB-C3B	-2.26	1.41	1.47
22	B	603	CLA	C1D-C2D	2.26	1.49	1.45
22	B	603	CLA	CHC-C1C	2.26	1.43	1.38
29	c	517	DGD	O3D-C3D	-2.26	1.37	1.43
26	a	414	LMG	O1-C1	2.26	1.44	1.40
26	c	518	LMG	C3-C2	2.25	1.58	1.52
22	b	608	CLA	CMA-C3A	-2.25	1.48	1.53
22	D	404	CLA	C4B-NB	2.25	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	H	103	DGD	C1G-C2G	2.25	1.57	1.50
22	a	405	CLA	CHC-C4B	-2.25	1.34	1.39
22	c	510	CLA	CMC-C2C	-2.25	1.46	1.50
22	C	507	CLA	C1B-C2B	2.25	1.48	1.43
22	B	601	CLA	CAC-C3C	-2.25	1.45	1.51
30	a	406	BCR	C1-C6	-2.24	1.50	1.53
29	C	517	DGD	O2G-C2G	-2.24	1.41	1.46
25	D	407	PL9	C2-C3	2.24	1.40	1.34
22	B	615	CLA	C1B-C2B	2.24	1.48	1.43
22	c	512	CLA	CMB-C2B	-2.23	1.46	1.50
22	c	507	CLA	CMC-C2C	-2.23	1.46	1.50
22	b	610	CLA	CMD-C2D	-2.23	1.46	1.50
28	a	411	LHG	C24-C23	2.23	1.57	1.50
22	B	603	CLA	C1B-NB	-2.23	1.34	1.37
26	D	408	LMG	O7-C8	-2.23	1.41	1.46
34	v	201	HEC	C3B-C2B	-2.22	1.32	1.36
22	B	607	CLA	CHC-C4B	-2.22	1.34	1.39
22	c	502	CLA	C1B-C2B	2.22	1.48	1.43
22	c	508	CLA	C1B-C2B	2.22	1.48	1.43
22	c	504	CLA	C3B-C4B	2.22	1.49	1.42
22	B	607	CLA	CMC-C2C	-2.22	1.46	1.50
22	B	613	CLA	C1D-ND	2.22	1.40	1.37
25	a	409	PL9	C6-C1	-2.22	1.44	1.48
22	B	610	CLA	CMB-C2B	-2.22	1.46	1.50
28	l	101	LHG	C6-C5	2.22	1.57	1.50
22	c	502	CLA	C4B-NB	2.22	1.40	1.37
22	a	405	CLA	CMC-C2C	-2.22	1.46	1.50
22	C	504	CLA	CHC-C4B	-2.22	1.34	1.39
30	b	618	BCR	C33-C5	-2.21	1.47	1.50
26	D	408	LMG	O4-C4	2.21	1.48	1.43
29	C	517	DGD	C2B-C1B	-2.21	1.44	1.50
22	C	513	CLA	CHC-C1C	2.21	1.42	1.38
25	a	409	PL9	C3-C4	-2.21	1.46	1.49
22	C	508	CLA	CMD-C2D	-2.21	1.46	1.50
22	A	403	CLA	CMC-C2C	-2.21	1.46	1.50
22	b	604	CLA	CMC-C2C	-2.20	1.46	1.50
22	d	404	CLA	CMA-C3A	-2.20	1.48	1.53
26	B	620	LMG	C11-C10	2.20	1.55	1.50
34	F	101	HEC	CMC-C2C	2.20	1.55	1.50
22	C	506	CLA	CAC-C3C	-2.20	1.45	1.51
22	d	405	CLA	O1D-CGD	2.20	1.26	1.21
22	b	609	CLA	C3B-C4B	2.20	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	402	CLA	C3B-C4B	2.20	1.49	1.42
22	C	504	CLA	CMD-C2D	-2.19	1.46	1.50
22	b	601	CLA	CHC-C1C	2.19	1.42	1.38
29	C	517	DGD	O1G-C1G	-2.19	1.40	1.45
22	b	609	CLA	CMD-C2D	-2.19	1.46	1.50
22	B	614	CLA	CMD-C2D	-2.19	1.46	1.50
22	C	501	CLA	C3B-C4B	2.19	1.49	1.42
22	c	501	CLA	CMD-C2D	-2.19	1.46	1.50
22	b	609	CLA	CMC-C2C	-2.19	1.46	1.50
22	C	505	CLA	C1B-C2B	2.19	1.48	1.43
28	d	409	LHG	P-O3	2.18	1.67	1.59
22	B	607	CLA	C1B-C2B	2.18	1.48	1.43
22	D	404	CLA	C3D-C4D	2.18	1.49	1.44
22	b	613	CLA	CMC-C2C	-2.18	1.46	1.50
22	B	601	CLA	CHC-C4B	-2.18	1.34	1.39
23	D	401	PHO	CBD-CGD	-2.18	1.49	1.52
22	A	405	CLA	CHC-C4B	-2.18	1.34	1.39
22	B	612	CLA	C3B-C4B	2.18	1.49	1.42
22	a	405	CLA	CMD-C2D	-2.18	1.46	1.50
22	c	501	CLA	CHC-C4B	-2.18	1.34	1.39
26	A	409	LMG	C4-C5	2.18	1.57	1.53
22	c	505	CLA	C1D-ND	2.18	1.40	1.37
22	b	606	CLA	CHC-C4B	-2.17	1.34	1.39
22	C	509	CLA	O2D-CGD	2.17	1.38	1.33
26	Y	101	LMG	O1-C1	2.17	1.43	1.40
22	b	616	CLA	MG-NB	2.17	2.10	2.05
25	d	407	PL9	C11-C9	-2.17	1.46	1.51
22	C	507	CLA	C3D-C4D	2.17	1.49	1.44
34	f	101	HEC	C2A-C3A	-2.17	1.32	1.36
22	B	603	CLA	MG-NC	2.16	2.11	2.06
22	B	615	CLA	C1D-C2D	2.16	1.49	1.45
28	D	413	LHG	C24-C23	2.16	1.57	1.50
22	B	606	CLA	CHC-C4B	-2.16	1.34	1.39
22	b	614	CLA	CMC-C2C	-2.16	1.46	1.50
22	B	607	CLA	O2A-CGA	2.16	1.39	1.33
22	a	402	CLA	C3B-C4B	2.16	1.49	1.42
29	A	413	DGD	C6D-C5D	2.16	1.58	1.51
22	b	602	CLA	CAC-C3C	-2.16	1.45	1.51
22	d	405	CLA	CHC-C4B	-2.15	1.34	1.39
23	A	404	PHO	CAC-C3C	-2.15	1.47	1.51
22	b	608	CLA	O2A-CGA	2.15	1.39	1.33
22	C	513	CLA	C1B-C2B	2.15	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	407	PL9	C15-C14	2.15	1.56	1.50
22	b	603	CLA	C1B-C2B	2.15	1.48	1.43
22	C	503	CLA	C3B-C4B	2.15	1.49	1.42
22	C	503	CLA	C1B-NB	-2.15	1.35	1.37
22	B	611	CLA	MG-NC	2.15	2.11	2.06
22	A	403	CLA	C1B-NB	-2.15	1.35	1.37
22	C	503	CLA	C1D-C2D	2.15	1.49	1.45
23	a	404	PHO	CMD-C2D	-2.15	1.47	1.51
28	D	410	LHG	C8-C7	-2.14	1.44	1.50
22	C	502	CLA	CMB-C2B	-2.14	1.46	1.50
22	c	510	CLA	CMD-C2D	-2.14	1.46	1.50
22	B	607	CLA	CMD-C2D	-2.14	1.46	1.50
22	B	602	CLA	CAB-C3B	-2.14	1.41	1.47
26	A	409	LMG	C1-C2	2.14	1.58	1.52
29	C	518	DGD	O2E-C2E	-2.14	1.37	1.43
22	B	612	CLA	CMB-C2B	-2.14	1.46	1.50
30	b	618	BCR	C36-C18	-2.14	1.46	1.50
30	D	406	BCR	C38-C26	-2.14	1.47	1.50
26	c	520	LMG	C4-C3	2.14	1.57	1.52
22	C	502	CLA	C1B-NB	-2.14	1.35	1.37
26	c	521	LMG	O1-C1	2.14	1.43	1.40
22	C	502	CLA	CMC-C2C	-2.14	1.46	1.50
22	b	614	CLA	C5-C3	-2.14	1.46	1.51
26	a	414	LMG	C7-C8	2.14	1.57	1.50
22	B	608	CLA	MG-NB	-2.14	2.01	2.05
31	j	101	STE	O1-C1	2.13	1.29	1.22
22	B	611	CLA	CMC-C2C	-2.13	1.46	1.50
26	a	414	LMG	C14-C13	2.13	1.62	1.51
22	b	607	CLA	C1A-CHA	-2.13	1.34	1.43
22	c	503	CLA	CAC-C3C	-2.13	1.45	1.51
22	B	611	CLA	C1C-NC	-2.13	1.34	1.37
22	C	511	CLA	CMD-C2D	-2.13	1.46	1.50
22	D	404	CLA	C3C-C2C	2.13	1.41	1.36
22	B	609	CLA	MG-ND	-2.13	2.01	2.05
22	c	506	CLA	C4B-NB	2.13	1.40	1.37
22	a	405	CLA	MG-NC	-2.13	2.01	2.06
28	a	411	LHG	P-O3	2.13	1.67	1.59
29	c	515	DGD	O3G-C3G	-2.13	1.40	1.43
22	C	513	CLA	CMC-C2C	-2.13	1.46	1.50
22	c	512	CLA	CMC-C2C	-2.13	1.46	1.50
22	c	512	CLA	C1D-C2D	2.13	1.49	1.45
22	B	615	CLA	C4B-NB	2.13	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	612	CLA	C1B-C2B	2.13	1.48	1.43
26	M	101	LMG	O6-C1	2.13	1.47	1.41
22	b	601	CLA	C3B-C4B	2.12	1.48	1.42
22	b	611	CLA	CAA-C2A	-2.12	1.50	1.54
22	C	502	CLA	C4B-NB	2.12	1.40	1.37
22	b	601	CLA	CMD-C2D	-2.12	1.46	1.50
22	b	613	CLA	C4B-NB	2.12	1.40	1.37
22	c	503	CLA	CHC-C1C	2.12	1.42	1.38
22	c	508	CLA	C4B-NB	2.12	1.40	1.37
23	D	401	PHO	C4D-CHA	2.12	1.42	1.39
26	B	620	LMG	C29-C28	2.11	1.55	1.50
22	b	606	CLA	O2A-CGA	2.11	1.39	1.33
22	c	509	CLA	CHC-C1C	2.11	1.42	1.38
26	m	101	LMG	C6-C5	2.11	1.58	1.51
22	d	403	CLA	CMD-C2D	-2.11	1.46	1.50
22	B	603	CLA	C1B-C2B	2.11	1.48	1.43
22	c	502	CLA	C3B-C4B	2.11	1.48	1.42
22	b	610	CLA	CMC-C2C	-2.11	1.46	1.50
29	A	413	DGD	C3D-C2D	2.11	1.57	1.52
28	d	408	LHG	C8-C7	-2.11	1.44	1.50
30	I	101	BCR	C4-C5	-2.11	1.47	1.51
22	B	609	CLA	CMD-C2D	-2.10	1.46	1.50
26	D	408	LMG	C7-C8	2.10	1.57	1.50
25	d	407	PL9	C16-C17	2.10	1.60	1.53
22	d	405	CLA	CMB-C2B	-2.10	1.46	1.50
22	C	510	CLA	CMB-C2B	-2.10	1.46	1.50
22	b	608	CLA	CMC-C2C	-2.10	1.46	1.50
22	C	510	CLA	O2A-CGA	2.10	1.39	1.33
30	T	101	BCR	C27-C26	-2.10	1.47	1.51
22	d	405	CLA	MG-ND	-2.10	2.01	2.05
22	c	501	CLA	C1B-NB	-2.10	1.35	1.37
22	c	510	CLA	CHC-C1C	2.10	1.42	1.38
22	C	509	CLA	C4B-NB	2.10	1.40	1.37
30	k	103	BCR	C27-C26	-2.10	1.47	1.51
29	c	517	DGD	C1D-C2D	2.10	1.58	1.52
22	b	608	CLA	C4B-NB	2.09	1.40	1.37
22	b	608	CLA	C1C-C2C	2.09	1.48	1.44
28	A	411	LHG	O7-C5	-2.09	1.41	1.46
29	H	103	DGD	O3G-C1D	2.09	1.43	1.40
22	b	611	CLA	CHC-C1C	2.09	1.42	1.38
22	c	503	CLA	C4B-NB	2.09	1.40	1.37
22	C	506	CLA	CMA-C3A	-2.09	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	601	CLA	CHB-C1B	2.09	1.44	1.39
26	c	521	LMG	C4-C3	2.08	1.57	1.52
30	T	101	BCR	C1-C6	-2.08	1.51	1.53
22	A	403	CLA	MG-NB	-2.08	2.01	2.05
22	B	601	CLA	CHC-C1C	2.08	1.42	1.38
22	b	601	CLA	C3D-C4D	2.08	1.48	1.44
22	B	606	CLA	C3D-C4D	2.08	1.48	1.44
22	B	605	CLA	C4B-NB	2.08	1.40	1.37
22	b	614	CLA	C4B-NB	2.08	1.40	1.37
22	C	508	CLA	MG-NC	-2.08	2.01	2.06
31	c	519	STE	C2-C1	2.08	1.55	1.50
25	D	407	PL9	C46-C44	-2.08	1.47	1.51
22	C	508	CLA	CMC-C2C	-2.08	1.46	1.50
27	A	410	SQD	O3-C3	-2.07	1.37	1.43
22	d	405	CLA	CMC-C2C	-2.07	1.46	1.50
22	b	615	CLA	CHC-C1C	2.07	1.42	1.38
22	b	605	CLA	C3B-C4B	2.07	1.48	1.42
22	C	513	CLA	CHC-C4B	-2.07	1.34	1.39
22	B	610	CLA	C1D-ND	2.07	1.40	1.37
22	B	604	CLA	C3B-C4B	2.07	1.48	1.42
29	C	516	DGD	C1G-C2G	2.07	1.57	1.50
28	D	411	LHG	C8-C7	-2.07	1.44	1.50
22	b	611	CLA	C1B-NB	-2.07	1.35	1.37
22	D	404	CLA	MG-NC	-2.06	2.01	2.06
22	b	616	CLA	C4B-NB	2.06	1.40	1.37
22	C	511	CLA	CMC-C2C	-2.06	1.46	1.50
29	c	516	DGD	O6D-C5D	-2.06	1.39	1.44
22	c	509	CLA	C3B-C4B	2.06	1.48	1.42
22	c	512	CLA	CMD-C2D	-2.06	1.46	1.50
29	c	515	DGD	C3G-C2G	2.06	1.57	1.50
34	f	101	HEC	C3B-C2B	-2.06	1.32	1.36
22	c	502	CLA	CHC-C4B	-2.06	1.34	1.39
22	D	403	CLA	C1A-CHA	-2.06	1.34	1.43
28	d	408	LHG	C3-C2	2.06	1.58	1.51
22	D	405	CLA	CAA-C2A	-2.06	1.50	1.54
22	C	505	CLA	C3B-C4B	2.06	1.48	1.42
22	B	602	CLA	CMA-C3A	-2.06	1.48	1.53
22	a	403	CLA	MG-ND	-2.06	2.01	2.05
22	b	605	CLA	C1A-CHA	-2.06	1.34	1.43
29	C	516	DGD	C2A-C1A	-2.06	1.44	1.50
22	B	607	CLA	CHC-C1C	2.06	1.42	1.38
22	B	608	CLA	CMC-C2C	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	405	CLA	C3B-C4B	2.06	1.48	1.42
22	C	511	CLA	CHC-C4B	-2.05	1.34	1.39
22	C	510	CLA	C1D-ND	2.05	1.40	1.37
22	B	606	CLA	CMB-C2B	-2.05	1.46	1.50
22	c	507	CLA	CMB-C2B	-2.05	1.46	1.50
22	c	508	CLA	CMC-C2C	-2.05	1.46	1.50
31	b	629	STE	C2-C1	2.05	1.55	1.50
22	B	612	CLA	MG-NB	2.05	2.09	2.05
22	D	404	CLA	O2D-CED	-2.05	1.40	1.45
22	D	405	CLA	CHC-C4B	-2.05	1.34	1.39
34	F	101	HEC	C3B-C2B	-2.05	1.32	1.36
22	C	506	CLA	O2D-CGD	2.04	1.38	1.33
25	d	407	PL9	C35-C34	-2.04	1.45	1.50
22	c	504	CLA	MG-NA	-2.04	2.01	2.06
22	B	602	CLA	MG-NA	2.04	2.11	2.06
22	c	511	CLA	CMB-C2B	-2.04	1.46	1.50
26	d	410	LMG	C35-C34	2.04	1.61	1.51
22	C	513	CLA	C3D-C4D	2.04	1.48	1.44
26	d	410	LMG	O2-C2	-2.04	1.37	1.43
22	C	507	CLA	CMD-C2D	-2.04	1.46	1.50
26	c	521	LMG	O6-C5	-2.04	1.39	1.44
22	C	513	CLA	C1D-C2D	2.04	1.49	1.45
30	x	101	BCR	C38-C26	-2.03	1.47	1.50
22	c	513	CLA	C1B-NB	-2.03	1.35	1.37
22	b	610	CLA	C1C-NC	-2.03	1.34	1.37
22	c	509	CLA	CMB-C2B	-2.03	1.46	1.50
27	f	102	SQD	O2-C2	-2.03	1.37	1.43
22	b	615	CLA	CAC-C3C	-2.03	1.45	1.51
22	B	602	CLA	CMC-C2C	-2.03	1.46	1.50
22	b	609	CLA	C3D-C4D	2.03	1.48	1.44
22	B	609	CLA	CAC-C3C	-2.03	1.45	1.51
22	c	510	CLA	C3B-C4B	2.02	1.48	1.42
26	c	518	LMG	O7-C10	2.02	1.39	1.35
22	b	605	CLA	CHC-C4B	-2.02	1.34	1.39
22	B	610	CLA	CAA-C2A	-2.02	1.50	1.54
25	A	408	PL9	C47-C48	2.02	1.56	1.50
22	C	509	CLA	C1B-C2B	2.02	1.47	1.43
22	C	501	CLA	C1B-NB	-2.02	1.35	1.37
22	b	607	CLA	C3B-C4B	2.02	1.48	1.42
30	b	617	BCR	C33-C5	-2.02	1.47	1.50
29	h	101	DGD	C4D-C3D	2.02	1.57	1.52
27	B	621	SQD	O2-C2	-2.02	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	618	BCR	C31-C1	-2.02	1.49	1.53
22	A	402	CLA	C3C-C2C	2.01	1.41	1.36
29	c	515	DGD	C4D-C3D	2.01	1.57	1.52
25	a	409	PL9	C25-C24	-2.01	1.45	1.50
22	c	507	CLA	CMD-C2D	-2.01	1.46	1.50
22	b	614	CLA	C1A-CHA	-2.01	1.34	1.43
30	D	406	BCR	C27-C26	-2.01	1.47	1.51
22	d	404	CLA	MG-ND	2.00	2.09	2.05
22	b	605	CLA	C3D-C4D	2.00	1.48	1.44
22	b	610	CLA	C1B-NB	-2.00	1.35	1.37
22	C	510	CLA	CAC-C3C	-2.00	1.46	1.51
22	C	506	CLA	C1B-NB	-2.00	1.35	1.37
22	a	403	CLA	CHC-C4B	-2.00	1.34	1.39
22	C	503	CLA	CMC-C2C	-2.00	1.46	1.50
22	c	504	CLA	CMB-C2B	-2.00	1.46	1.50
26	B	620	LMG	C16-C15	2.00	1.61	1.51
34	v	201	HEC	CHD-C4C	-2.00	1.34	1.39

All (1412) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	101	SQD	O6-C1-C2	10.62	124.41	108.27
22	C	510	CLA	C4A-NA-C1A	10.25	111.35	106.68
22	C	503	CLA	C4A-NA-C1A	9.78	111.14	106.68
22	C	511	CLA	C4A-NA-C1A	9.02	110.80	106.68
22	H	101	CLA	C4A-NA-C1A	8.96	110.77	106.68
22	c	511	CLA	C4A-NA-C1A	8.66	110.63	106.68
22	b	601	CLA	C4A-NA-C1A	8.19	110.42	106.68
22	C	501	CLA	C4A-NA-C1A	8.07	110.36	106.68
22	c	501	CLA	C4A-NA-C1A	7.84	110.25	106.68
22	a	402	CLA	C4A-NA-C1A	7.74	110.21	106.68
22	B	609	CLA	C4A-NA-C1A	7.70	110.19	106.68
22	B	603	CLA	C4A-NA-C1A	7.62	110.16	106.68
22	B	614	CLA	C4A-NA-C1A	7.37	110.04	106.68
22	C	502	CLA	C4A-NA-C1A	7.12	109.93	106.68
22	C	507	CLA	C4A-NA-C1A	7.11	109.92	106.68
22	B	606	CLA	C4A-NA-C1A	6.83	109.80	106.68
22	B	615	CLA	C4A-NA-C1A	6.82	109.79	106.68
22	B	605	CLA	C4A-NA-C1A	6.67	109.72	106.68
27	B	621	SQD	O6-C1-C2	6.44	118.06	108.27
22	b	606	CLA	C4A-NA-C1A	6.35	109.58	106.68
22	C	513	CLA	C4A-NA-C1A	6.21	109.51	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	404	CLA	C4A-NA-C1A	6.21	109.51	106.68
22	B	608	CLA	C4A-NA-C1A	6.18	109.50	106.68
22	b	603	CLA	O2D-CGD-O1D	-6.17	111.84	123.85
27	a	410	SQD	O6-C1-C2	6.08	117.51	108.27
22	c	507	CLA	C4A-NA-C1A	6.07	109.45	106.68
23	d	401	PHO	C4D-CHA-CBD	-6.05	105.56	108.45
22	b	608	CLA	C3B-C4B-NB	-5.92	105.25	110.53
22	b	603	CLA	C4A-NA-C1A	5.85	109.35	106.68
22	c	510	CLA	C4A-NA-C1A	5.75	109.30	106.68
22	b	616	CLA	O2D-CGD-O1D	-5.67	112.81	123.85
22	d	403	CLA	C4A-NA-C1A	5.66	109.26	106.68
22	b	606	CLA	O2D-CGD-O1D	-5.63	112.89	123.85
22	b	615	CLA	C4A-NA-C1A	5.56	109.22	106.68
22	A	402	CLA	C4A-NA-C1A	5.56	109.22	106.68
22	b	603	CLA	O2D-CGD-CBD	5.56	120.95	111.23
22	c	509	CLA	C4A-NA-C1A	5.52	109.20	106.68
22	a	403	CLA	C4A-NA-C1A	5.50	109.19	106.68
27	f	102	SQD	O6-C1-C2	5.47	116.58	108.27
22	b	612	CLA	C4A-NA-C1A	5.44	109.16	106.68
22	c	501	CLA	O2D-CGD-O1D	-5.43	113.28	123.85
22	c	513	CLA	C4A-NA-C1A	5.33	109.11	106.68
29	H	103	DGD	O3G-C3G-C2G	-5.30	97.93	110.82
22	B	604	CLA	O2D-CGD-O1D	-5.26	113.60	123.85
22	b	602	CLA	O2D-CGD-CBD	5.26	120.42	111.23
22	B	602	CLA	O2D-CGD-O1D	-5.25	113.64	123.85
23	a	404	PHO	C2B-C1B-NB	-5.17	105.69	109.43
27	t	102	SQD	O47-C7-C8	5.14	122.60	111.48
23	A	404	PHO	C4D-CHA-CBD	-5.10	106.01	108.45
27	A	410	SQD	O6-C1-C2	5.10	116.01	108.27
27	B	621	SQD	O47-C7-C8	5.08	122.47	111.48
34	f	101	HEC	CBD-CAD-C3D	-5.06	98.53	112.53
27	D	409	SQD	O6-C1-C2	5.04	115.93	108.27
22	C	513	CLA	O2D-CGD-O1D	-5.04	114.03	123.85
22	b	616	CLA	C4A-NA-C1A	5.04	108.98	106.68
22	c	506	CLA	C4A-NA-C1A	5.03	108.98	106.68
22	B	611	CLA	C4A-NA-C1A	5.03	108.97	106.68
22	b	605	CLA	C4A-NA-C1A	5.01	108.96	106.68
27	D	409	SQD	O8-S-C6	4.99	115.60	105.97
22	B	610	CLA	O2D-CGD-CBD	4.97	119.91	111.23
22	C	512	CLA	C4A-NA-C1A	4.92	108.92	106.68
33	D	402	BCT	O2-C-O1	4.91	132.25	119.68
26	b	622	LMG	C1-O6-C5	-4.91	104.14	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	601	CLA	O2D-CGD-CBD	4.90	119.79	111.23
27	f	102	SQD	O9-S-C6	4.89	114.06	106.76
22	b	611	CLA	C4A-NA-C1A	4.87	108.90	106.68
25	a	409	PL9	C7-C3-C4	4.86	120.91	116.91
22	b	614	CLA	C4A-NA-C1A	4.85	108.89	106.68
22	c	508	CLA	C4A-NA-C1A	4.83	108.88	106.68
27	A	410	SQD	O7-S-C6	4.82	113.95	106.76
23	d	401	PHO	C2B-C1B-NB	-4.81	105.96	109.43
22	B	610	CLA	O2D-CGD-O1D	-4.77	114.56	123.85
22	b	605	CLA	O2D-CGD-O1D	-4.76	114.57	123.85
22	b	613	CLA	C4A-NA-C1A	4.75	108.85	106.68
22	d	404	CLA	C1D-ND-C4D	4.73	109.63	106.31
22	b	612	CLA	O2A-CGA-O1A	-4.71	111.85	123.63
22	C	506	CLA	C4A-NA-C1A	4.67	108.81	106.68
27	A	410	SQD	O47-C7-C8	4.67	121.59	111.48
22	b	602	CLA	O2D-CGD-O1D	-4.67	114.76	123.85
22	D	404	CLA	C4A-NA-C1A	4.65	108.80	106.68
22	c	505	CLA	O2D-CGD-O1D	-4.62	114.86	123.85
22	C	508	CLA	C4A-NA-C1A	4.61	108.78	106.68
22	c	512	CLA	C3B-C4B-NB	-4.61	106.42	110.53
27	D	409	SQD	O9-S-C6	4.60	113.63	106.76
22	b	604	CLA	C1-C2-C3	-4.58	118.69	126.20
23	A	404	PHO	C3B-C4B-NB	-4.58	104.48	107.46
27	f	102	SQD	O7-S-C6	4.58	113.59	106.76
22	A	403	CLA	C4A-NA-C1A	4.55	108.75	106.68
22	c	509	CLA	O2A-CGA-O1A	-4.54	112.26	123.63
29	h	101	DGD	C3D-C4D-C5D	-4.53	102.02	110.23
28	D	411	LHG	O4-P-O5	4.52	133.49	112.44
30	c	514	BCR	C35-C13-C14	-4.50	115.53	122.82
29	C	518	DGD	O3G-C3G-C2G	-4.49	99.90	110.82
27	A	412	SQD	C45-O47-C7	4.46	124.22	117.78
28	A	411	LHG	O4-P-O5	4.46	133.19	112.44
27	B	621	SQD	O7-S-C6	4.46	113.41	106.76
22	b	609	CLA	C4A-NA-C1A	4.46	108.71	106.68
22	b	613	CLA	O2D-CGD-O1D	-4.44	115.21	123.85
27	A	410	SQD	O9-S-O7	-4.44	99.39	113.82
22	B	604	CLA	O1D-CGD-CBD	4.42	133.23	124.52
22	c	502	CLA	C4A-NA-C1A	4.38	108.68	106.68
25	D	407	PL9	C7-C3-C4	4.37	120.51	116.91
23	A	404	PHO	C2B-C1B-NB	-4.35	106.28	109.43
28	b	623	LHG	O4-P-O5	4.35	132.68	112.44
22	B	609	CLA	O2D-CGD-O1D	-4.34	115.39	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	101	SQD	C1-C2-C3	-4.34	100.88	110.01
34	F	101	HEC	C1D-ND-C4D	4.33	110.34	105.21
22	B	603	CLA	O2A-CGA-O1A	-4.33	112.80	123.63
22	C	512	CLA	CHB-C4A-NA	4.32	130.64	124.40
28	D	413	LHG	O4-P-O5	4.28	132.36	112.44
27	A	410	SQD	C46-C45-C44	-4.26	101.86	111.78
30	b	617	BCR	C2-C1-C6	4.25	116.61	110.44
27	L	101	SQD	C45-O47-C7	4.25	127.96	117.80
22	b	610	CLA	C4A-NA-C1A	4.23	108.61	106.68
22	c	507	CLA	O2D-CGD-O1D	-4.21	115.66	123.85
27	B	621	SQD	C3-C4-C5	4.21	117.86	110.23
26	m	101	LMG	O3-C3-C2	-4.20	100.47	110.38
34	f	101	HEC	CAB-C3B-C4B	4.20	130.25	124.79
22	b	602	CLA	C4A-NA-C1A	4.19	108.59	106.68
22	B	601	CLA	O2D-CGD-O1D	-4.19	115.70	123.85
28	a	411	LHG	O4-P-O5	4.18	131.90	112.44
28	d	408	LHG	O4-P-O5	4.18	131.87	112.44
22	c	505	CLA	O2D-CGD-CBD	4.16	118.50	111.23
23	a	404	PHO	C4D-CHA-CBD	-4.14	106.47	108.45
22	b	615	CLA	CHB-C1B-NB	4.14	130.26	124.05
26	b	622	LMG	O1-C1-C2	-4.12	102.01	108.27
30	B	617	BCR	C29-C30-C25	4.12	116.42	110.44
30	B	618	BCR	C29-C30-C25	4.12	116.42	110.44
28	D	410	LHG	O4-P-O5	4.11	131.55	112.44
33	d	402	BCT	O2-C-O1	4.10	130.17	119.68
30	B	616	BCR	C2-C1-C6	4.08	116.37	110.44
27	f	102	SQD	O9-S-O7	-4.05	100.64	113.82
22	B	610	CLA	CMB-C2B-C1B	-4.04	119.26	125.42
22	c	512	CLA	C4A-NA-C1A	4.03	108.52	106.68
23	D	401	PHO	C2B-C1B-NB	-4.02	106.52	109.43
22	C	512	CLA	O2D-CGD-O1D	-4.02	116.02	123.85
28	l	101	LHG	O4-P-O5	4.01	131.09	112.44
25	a	409	PL9	C7-C3-C2	-4.01	118.67	123.39
22	b	604	CLA	C4A-NA-C1A	3.98	108.50	106.68
27	t	102	SQD	O48-C23-O10	-3.98	113.67	123.63
31	L	103	STE	O2-C1-C2	3.98	126.57	114.00
25	A	408	PL9	C7-C3-C4	3.98	120.19	116.91
22	b	616	CLA	O1D-CGD-CBD	3.97	132.34	124.52
27	L	101	SQD	O48-C23-C24	3.96	123.92	111.83
29	c	516	DGD	O3G-C3G-C2G	-3.96	101.18	110.82
23	d	401	PHO	O1D-CGD-CBD	3.95	130.71	124.72
28	d	409	LHG	O4-P-O5	3.95	130.80	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	517	DGD	O3G-C3G-C2G	-3.93	101.25	110.82
22	a	405	CLA	CHB-C4A-NA	3.93	130.07	124.40
22	c	509	CLA	O2D-CGD-O1D	-3.93	116.21	123.85
27	a	410	SQD	C1-C2-C3	-3.92	101.75	110.01
22	A	402	CLA	CHB-C4A-NA	3.90	130.03	124.40
27	a	410	SQD	C1-O5-C5	-3.88	106.14	113.72
27	L	101	SQD	O5-C5-C4	3.88	116.69	109.70
25	A	408	PL9	O1-C4-C3	-3.88	116.64	120.73
23	D	401	PHO	C4D-CHA-CBD	-3.87	106.60	108.45
25	d	407	PL9	C22-C23-C24	-3.87	118.77	127.62
28	L	102	LHG	O4-P-O5	3.87	130.43	112.44
27	a	410	SQD	O8-S-C6	3.86	113.42	105.97
22	c	512	CLA	C1-C2-C3	-3.85	119.89	126.20
22	B	613	CLA	CHC-C4B-NB	3.84	129.81	124.05
22	C	501	CLA	C3B-C4B-NB	-3.84	107.10	110.53
30	B	618	BCR	C38-C26-C25	-3.84	120.30	124.48
22	B	613	CLA	C4A-NA-C1A	3.84	108.43	106.68
22	c	512	CLA	O2D-CGD-O1D	-3.84	116.38	123.85
22	b	614	CLA	O2D-CGD-O1D	-3.81	116.44	123.85
22	a	402	CLA	O1D-CGD-CBD	3.80	132.02	124.52
30	C	514	BCR	C33-C5-C6	-3.80	120.33	124.48
22	a	403	CLA	CHB-C4A-NA	3.80	129.88	124.40
27	A	410	SQD	C45-O47-C7	3.80	126.88	117.80
23	D	401	PHO	C3B-C4B-NB	-3.78	105.00	107.46
22	C	510	CLA	C3B-C4B-NB	-3.77	107.16	110.53
29	C	516	DGD	O1G-C1A-C2A	-3.76	100.37	111.83
23	A	404	PHO	C1-C2-C3	-3.74	120.07	126.20
22	C	505	CLA	C3B-C4B-NB	-3.73	107.20	110.53
27	B	621	SQD	O48-C23-C24	3.72	123.19	111.83
27	A	410	SQD	C1-O5-C5	-3.72	106.45	113.72
34	v	201	HEC	C1D-ND-C4D	3.72	109.61	105.21
22	c	506	CLA	C2D-C1D-ND	-3.72	106.45	110.13
25	A	408	PL9	C22-C23-C24	-3.72	119.11	127.62
34	v	201	HEC	C1D-C2D-C3D	-3.72	103.07	106.98
26	A	409	LMG	O6-C1-O1	-3.72	101.27	110.04
22	b	609	CLA	C3B-C4B-NB	-3.71	107.22	110.53
34	V	201	HEC	C1D-ND-C4D	3.70	109.59	105.21
26	c	521	LMG	C1-O6-C5	-3.70	106.50	113.72
22	B	603	CLA	O2D-CGD-O1D	-3.69	116.66	123.85
22	A	405	CLA	O2D-CGD-CBD	3.69	117.69	111.23
30	k	103	BCR	C39-C30-C25	-3.69	104.46	110.24
22	b	604	CLA	C4-C3-C5	3.67	121.60	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	509	CLA	C4A-NA-C1A	3.67	108.35	106.68
25	D	407	PL9	C36-C34-C33	-3.66	112.94	121.17
31	B	625	STE	O2-C1-C2	3.66	125.56	114.00
30	x	101	BCR	C27-C26-C25	3.65	127.64	122.70
22	A	403	CLA	O2D-CGD-O1D	-3.65	116.74	123.85
30	K	101	BCR	C7-C8-C9	-3.65	120.84	126.23
22	B	602	CLA	C6-C7-C8	-3.65	103.84	115.97
22	C	506	CLA	C3B-C4B-NB	-3.65	107.28	110.53
30	T	101	BCR	C27-C26-C25	3.63	127.61	122.70
25	D	407	PL9	C40-C39-C41	3.62	121.51	115.23
22	B	603	CLA	CHB-C4A-NA	3.62	129.62	124.40
29	C	518	DGD	C4D-C3D-C2D	-3.62	104.48	110.83
22	B	609	CLA	CHB-C4A-NA	3.61	129.62	124.40
22	d	404	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
22	b	613	CLA	CHB-C4A-NA	3.61	129.61	124.40
34	F	101	HEC	CBD-CAD-C3D	-3.60	102.57	112.53
22	b	607	CLA	C4A-NA-C1A	3.60	108.32	106.68
22	b	605	CLA	O1D-CGD-CBD	3.59	131.61	124.52
22	c	510	CLA	C3B-C4B-NB	-3.59	107.32	110.53
27	L	101	SQD	O5-C1-C2	-3.59	102.99	110.37
27	A	412	SQD	O47-C7-C8	3.59	119.25	111.48
22	B	613	CLA	C3B-C4B-NB	-3.59	107.33	110.53
30	C	514	BCR	C7-C8-C9	-3.58	120.94	126.23
22	c	509	CLA	CHB-C4A-NA	3.57	129.55	124.40
22	d	404	CLA	O2D-CGD-O1D	-3.56	116.91	123.85
26	m	101	LMG	O7-C10-O9	-3.56	115.37	123.70
23	a	404	PHO	O2D-CGD-CBD	3.56	114.86	110.95
22	A	402	CLA	CHD-C1D-ND	-3.56	119.79	124.80
22	B	610	CLA	C1-C2-C3	-3.56	120.36	126.20
22	C	509	CLA	O2D-CGD-O1D	-3.56	116.93	123.85
22	a	405	CLA	O2A-CGA-O1A	-3.55	114.74	123.63
22	C	503	CLA	C3B-C4B-NB	-3.55	107.36	110.53
22	b	611	CLA	O2D-CGD-O1D	-3.55	116.95	123.85
34	v	201	HEC	CMD-C2D-C1D	3.54	130.57	125.03
30	d	406	BCR	C38-C26-C25	-3.54	120.62	124.48
30	I	101	BCR	C27-C26-C25	3.53	127.48	122.70
25	A	408	PL9	C36-C34-C33	-3.53	113.24	121.17
22	C	505	CLA	CHB-C4A-NA	3.52	129.48	124.40
22	C	504	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
30	K	101	BCR	C15-C16-C17	-3.52	116.32	123.52
27	A	410	SQD	C1-C2-C3	-3.52	102.61	110.01
22	B	612	CLA	CHA-C1A-NA	-3.51	118.44	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	t	102	SQD	O48-C23-C24	3.51	122.53	111.83
22	A	405	CLA	O2D-CGD-O1D	-3.50	117.03	123.85
22	b	606	CLA	O2D-CGD-CBD	3.50	117.35	111.23
22	A	405	CLA	C4A-NA-C1A	3.50	108.27	106.68
22	c	503	CLA	O2D-CGD-O1D	-3.50	117.04	123.85
29	c	517	DGD	O3G-C3G-C2G	-3.49	102.33	110.82
22	b	605	CLA	CHD-C1D-ND	-3.49	119.89	124.80
22	B	614	CLA	CHC-C4B-NB	3.48	129.27	124.05
29	h	101	DGD	C4D-C3D-C2D	-3.47	104.74	110.83
29	c	517	DGD	C3D-C4D-C5D	-3.47	103.94	110.23
31	C	519	STE	O2-C1-O1	-3.45	114.46	123.33
22	B	613	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
22	B	610	CLA	C4A-NA-C1A	3.45	108.25	106.68
30	t	101	BCR	C7-C8-C9	-3.44	121.14	126.23
22	d	404	CLA	C3B-C4B-NB	-3.44	107.46	110.53
30	T	101	BCR	C7-C8-C9	-3.44	121.15	126.23
22	b	613	CLA	O2D-CGD-CBD	3.43	117.23	111.23
22	b	611	CLA	CHD-C1D-ND	-3.43	119.97	124.80
27	D	409	SQD	O48-C23-C24	3.43	122.28	111.83
34	V	201	HEC	CHB-C4A-NA	3.42	128.18	124.45
22	c	501	CLA	O2D-CGD-CBD	3.42	117.21	111.23
30	D	406	BCR	C7-C8-C9	-3.41	121.18	126.23
22	C	507	CLA	O2D-CGD-O1D	-3.41	117.20	123.85
27	a	410	SQD	O9-S-C6	3.41	111.85	106.76
27	D	409	SQD	O8-S-O9	-3.41	102.87	111.40
22	c	512	CLA	CHB-C4A-NA	3.41	129.32	124.40
25	d	407	PL9	C37-C38-C39	-3.40	119.83	127.62
22	b	614	CLA	C3B-C4B-NB	-3.40	107.49	110.53
34	F	101	HEC	CAC-C3C-C4C	3.40	129.59	124.91
28	D	413	LHG	O8-C23-C24	3.40	122.20	111.83
26	m	101	LMG	O1-C7-C8	-3.39	102.57	110.82
22	c	508	CLA	C3B-C4B-NB	-3.38	107.51	110.53
29	c	516	DGD	O6D-C1D-O3G	-3.37	102.07	110.04
22	C	502	CLA	O1D-CGD-CBD	3.37	131.16	124.52
22	D	405	CLA	O2D-CGD-O1D	-3.37	117.30	123.85
27	L	101	SQD	O47-C7-C8	3.36	118.76	111.48
22	c	513	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
22	A	402	CLA	C1D-ND-C4D	-3.35	103.96	106.31
30	D	406	BCR	C2-C1-C6	3.35	115.31	110.44
22	b	602	CLA	O2A-CGA-O1A	-3.35	115.25	123.63
22	c	510	CLA	CHB-C4A-NA	3.34	129.22	124.40
26	M	101	LMG	C4-C3-C2	-3.33	104.98	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	518	LMG	O6-C1-O1	-3.33	102.17	110.04
22	D	403	CLA	O2A-CGA-O1A	-3.33	115.30	123.63
22	C	509	CLA	C3B-C4B-NB	-3.33	107.56	110.53
30	k	102	BCR	C2-C1-C6	3.32	115.27	110.44
22	b	612	CLA	CAC-C3C-C4C	3.32	129.11	124.79
27	f	102	SQD	C1-C2-C3	-3.30	103.06	110.01
25	D	407	PL9	C22-C23-C24	-3.30	120.07	127.62
34	f	101	HEC	CAB-C3B-C2B	-3.30	121.50	127.56
30	k	101	BCR	C15-C14-C13	-3.30	122.65	127.28
28	D	413	LHG	O8-C23-O10	-3.30	115.38	123.63
30	c	514	BCR	C27-C26-C25	3.29	127.16	122.70
25	D	407	PL9	C50-C49-C48	-3.29	112.78	122.66
22	C	510	CLA	CHB-C4A-NA	3.28	129.14	124.40
26	m	101	LMG	O6-C1-O1	-3.28	102.29	110.04
27	L	101	SQD	O2-C2-C1	3.28	117.89	110.08
22	b	611	CLA	O2D-CGD-CBD	3.28	116.96	111.23
29	c	515	DGD	O6D-C1D-O3G	-3.27	102.31	110.04
22	b	614	CLA	O2A-CGA-O1A	-3.27	115.45	123.63
22	c	513	CLA	C1-C2-C3	-3.27	120.84	126.20
22	B	612	CLA	CHB-C4A-NA	3.27	129.11	124.40
22	c	507	CLA	O2A-CGA-O1A	-3.26	115.46	123.63
26	d	410	LMG	O6-C1-O1	-3.26	102.33	110.04
22	c	502	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
30	B	618	BCR	C2-C1-C6	3.26	115.18	110.44
30	B	618	BCR	C15-C14-C13	-3.26	122.71	127.28
22	b	609	CLA	O1D-CGD-CBD	3.25	130.93	124.52
30	I	101	BCR	C40-C30-C25	3.25	115.34	110.24
22	d	404	CLA	O2D-CGD-CBD	3.25	116.91	111.23
22	C	513	CLA	O1D-CGD-CBD	3.25	130.92	124.52
31	B	622	STE	C3-C2-C1	-3.24	106.04	114.51
22	b	613	CLA	CAC-C3C-C4C	3.24	129.01	124.79
29	H	103	DGD	O2D-C2D-C1D	-3.24	102.36	110.08
22	b	612	CLA	CHB-C4A-NA	3.24	129.07	124.40
22	c	503	CLA	C4A-NA-C1A	3.24	108.16	106.68
22	c	508	CLA	O2A-CGA-O1A	-3.23	115.54	123.63
22	b	604	CLA	C3B-C4B-NB	-3.22	107.65	110.53
23	d	401	PHO	O2D-CGD-O1D	-3.22	117.58	123.85
27	f	102	SQD	O48-C23-O10	-3.22	115.58	123.63
26	D	408	LMG	C3-C4-C5	-3.21	104.41	110.23
27	a	410	SQD	O9-S-O7	-3.21	103.38	113.82
22	b	603	CLA	CHB-C1B-NB	3.21	128.87	124.05
23	d	401	PHO	CMB-C2B-C3B	3.21	131.10	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	401	PHO	O1D-CGD-CBD	3.21	129.59	124.72
22	C	507	CLA	CHB-C4A-NA	3.21	129.03	124.40
22	C	508	CLA	CHD-C1D-ND	-3.20	120.29	124.80
22	B	607	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
22	c	506	CLA	CHB-C4A-NA	3.20	129.02	124.40
22	c	512	CLA	CHD-C4C-NC	3.20	129.19	124.23
22	A	403	CLA	CMB-C2B-C1B	-3.20	120.55	125.42
34	v	201	HEC	CAB-C3B-C4B	3.19	128.94	124.79
22	d	404	CLA	C2B-C1B-NB	-3.19	107.02	110.33
22	b	603	CLA	CED-O2D-CGD	-3.19	108.69	115.92
22	b	610	CLA	C6-C5-C3	3.19	121.23	113.47
27	B	621	SQD	C1-O5-C5	-3.18	107.51	113.72
22	b	609	CLA	CHB-C1B-NB	3.18	128.82	124.05
23	d	401	PHO	C3D-C4D-ND	3.18	111.78	107.71
22	C	501	CLA	O2D-CGD-O1D	-3.17	117.69	123.85
22	D	403	CLA	C1-C2-C3	-3.16	121.02	126.20
22	b	605	CLA	CHB-C4A-NA	3.16	128.96	124.40
28	a	411	LHG	O8-C23-C24	3.15	121.45	111.83
34	v	201	HEC	CBD-CAD-C3D	-3.15	103.81	112.53
23	A	404	PHO	C5-C3-C2	3.15	128.24	121.17
30	C	514	BCR	C15-C16-C17	-3.15	117.08	123.52
22	B	611	CLA	C11-C12-C13	-3.14	105.53	115.97
22	D	404	CLA	C3B-C4B-NB	-3.14	107.73	110.53
30	a	406	BCR	C27-C26-C25	3.14	126.94	122.70
25	D	407	PL9	C30-C29-C31	-3.13	109.79	115.23
30	I	101	BCR	C11-C10-C9	-3.13	122.88	127.28
30	K	101	BCR	C11-C10-C9	-3.13	122.89	127.28
22	b	615	CLA	C3B-C4B-NB	-3.13	107.74	110.53
27	A	410	SQD	O5-C5-C4	3.13	115.33	109.70
30	k	101	BCR	C24-C23-C22	-3.12	121.61	126.23
22	C	510	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
30	b	619	BCR	C29-C30-C25	3.12	114.97	110.44
29	c	516	DGD	C3D-C4D-C5D	-3.12	104.58	110.23
30	H	102	BCR	C2-C1-C6	3.12	114.97	110.44
27	f	102	SQD	C1-O5-C5	-3.12	107.64	113.72
27	L	101	SQD	O47-C45-C46	3.11	119.50	108.34
29	H	103	DGD	C1D-C2D-C3D	-3.10	103.48	110.01
30	B	617	BCR	C37-C22-C21	-3.10	117.79	122.82
29	A	413	DGD	O6E-C5E-C4E	3.10	115.29	109.70
22	A	402	CLA	O1D-CGD-CBD	3.10	130.62	124.52
22	b	610	CLA	CHB-C4A-NA	3.09	128.86	124.40
22	b	608	CLA	CHB-C4A-NA	3.09	128.86	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	603	CLA	O2A-CGA-O1A	-3.09	115.91	123.63
29	C	518	DGD	O6D-C1D-O3G	-3.09	102.75	110.04
22	B	602	CLA	C4-C3-C5	3.09	120.58	115.23
22	b	602	CLA	CHB-C4A-NA	3.09	128.85	124.40
31	L	103	STE	O1-C1-C2	-3.08	113.31	123.09
22	c	507	CLA	O2D-CGD-CBD	3.08	116.61	111.23
25	A	408	PL9	C7-C3-C2	-3.08	119.76	123.39
26	M	101	LMG	O6-C1-O1	-3.08	102.77	110.04
22	A	405	CLA	CHD-C1D-ND	-3.08	120.47	124.80
27	a	410	SQD	O47-C7-O49	-3.07	116.53	123.70
22	a	403	CLA	CED-O2D-CGD	-3.07	108.95	115.92
30	K	102	BCR	C27-C26-C25	3.06	126.84	122.70
22	c	501	CLA	CED-O2D-CGD	-3.06	108.98	115.92
26	m	101	LMG	O1-C1-C2	-3.05	103.64	108.27
22	a	403	CLA	O2A-CGA-O1A	-3.05	116.00	123.63
22	C	509	CLA	C1-O2A-CGA	3.05	124.03	116.65
22	b	611	CLA	CHD-C1D-C2D	3.05	131.83	125.49
26	b	622	LMG	O2-C2-C1	-3.04	102.83	110.08
22	C	502	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
29	c	516	DGD	C3E-C4E-C5E	-3.04	104.72	110.23
22	B	610	CLA	C1C-C2C-C3C	-3.04	103.78	106.98
27	B	621	SQD	O48-C23-O10	-3.04	116.03	123.63
30	d	406	BCR	C27-C26-C25	3.03	126.80	122.70
23	a	404	PHO	OBD-CAD-CBD	-3.03	121.38	125.82
22	b	604	CLA	CHB-C4A-NA	3.03	128.77	124.40
22	B	615	CLA	CHB-C4A-NA	3.03	128.77	124.40
22	B	612	CLA	O1D-CGD-CBD	3.03	130.49	124.52
30	d	406	BCR	C3-C4-C5	-3.03	108.66	114.06
22	c	504	CLA	C4A-NA-C1A	3.03	108.06	106.68
22	C	506	CLA	C4-C3-C5	3.03	120.48	115.23
22	B	609	CLA	CHD-C1D-ND	-3.02	120.55	124.80
29	C	518	DGD	O5D-C6D-C5D	-3.02	102.61	109.42
29	H	103	DGD	C3E-C4E-C5E	-3.02	104.75	110.23
30	H	102	BCR	C24-C23-C22	-3.02	121.77	126.23
30	K	101	BCR	C27-C26-C25	3.01	126.77	122.70
22	c	512	CLA	CHD-C1D-ND	-3.01	120.56	124.80
28	b	623	LHG	C11-C10-C9	-3.01	99.15	114.37
25	a	409	PL9	C37-C38-C39	-3.01	120.74	127.62
22	b	601	CLA	CHB-C4A-NA	3.01	128.74	124.40
22	B	610	CLA	CHB-C4A-NA	3.00	128.73	124.40
27	A	410	SQD	O9-S-C6	3.00	111.23	106.76
22	c	510	CLA	O2D-CGD-O1D	-3.00	118.01	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404	PHO	CMB-C2B-C3B	3.00	130.68	124.68
34	V	201	HEC	CAD-CBD-CGD	-3.00	105.71	113.67
22	C	512	CLA	C1-C2-C3	-3.00	121.29	126.20
22	c	509	CLA	CHD-C1D-ND	-3.00	120.59	124.80
22	c	506	CLA	C1D-ND-C4D	2.99	108.41	106.31
22	b	616	CLA	CHB-C4A-NA	2.99	128.72	124.40
34	v	201	HEC	C2A-C1A-NA	-2.99	107.44	110.32
22	B	602	CLA	O2D-CGD-CBD	2.99	116.45	111.23
30	B	618	BCR	C36-C18-C17	-2.98	117.98	122.82
22	B	609	CLA	O2A-CGA-O1A	-2.98	116.16	123.63
22	C	501	CLA	C4-C3-C5	2.98	120.40	115.23
29	C	516	DGD	O6D-C1D-O3G	-2.98	103.00	110.04
22	b	608	CLA	O2D-CGD-CBD	2.98	116.44	111.23
29	c	517	DGD	O6D-C1D-O3G	-2.98	103.01	110.04
27	A	410	SQD	O48-C23-C24	2.97	120.90	111.83
27	L	101	SQD	O7-S-C6	2.97	111.19	106.76
29	C	517	DGD	C1D-C2D-C3D	-2.97	103.76	110.01
30	K	102	BCR	C8-C7-C6	-2.96	119.09	127.00
26	a	414	LMG	C7-O1-C1	2.96	120.14	113.80
30	k	101	BCR	C15-C16-C17	-2.96	117.47	123.52
22	B	615	CLA	C2C-C1C-NC	2.96	113.09	109.98
27	L	101	SQD	O9-S-C6	2.95	111.17	106.76
25	d	407	PL9	C40-C39-C41	2.95	120.35	115.23
27	B	621	SQD	C46-C45-C44	-2.95	104.90	111.78
22	C	504	CLA	O2A-CGA-O1A	-2.95	116.24	123.63
22	c	506	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
22	C	501	CLA	O2D-CGD-CBD	2.95	116.38	111.23
30	k	101	BCR	C7-C8-C9	-2.94	121.88	126.23
22	C	509	CLA	CHB-C4A-NA	2.94	128.64	124.40
31	C	519	STE	O2-C1-C2	2.94	123.28	114.00
22	C	503	CLA	C4-C3-C5	2.94	120.33	115.23
30	b	617	BCR	C27-C26-C25	2.93	126.67	122.70
22	d	405	CLA	O2A-CGA-O1A	-2.93	116.30	123.63
30	b	617	BCR	C38-C26-C25	-2.92	121.29	124.48
23	D	401	PHO	C1-C2-C3	-2.92	121.41	126.20
22	a	403	CLA	CAC-C3C-C4C	2.92	128.59	124.79
22	B	608	CLA	C2C-C1C-NC	2.92	113.05	109.98
30	c	514	BCR	C2-C1-C6	2.92	114.68	110.44
22	c	508	CLA	CHD-C1D-ND	-2.92	120.69	124.80
22	D	403	CLA	C4-C3-C5	2.92	120.29	115.23
22	H	101	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
30	c	514	BCR	C30-C25-C26	-2.91	118.65	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	614	CLA	CHB-C4A-NA	2.91	128.60	124.40
22	B	611	CLA	O2A-CGA-O1A	-2.91	116.34	123.63
22	b	614	CLA	CMB-C2B-C1B	-2.91	120.99	125.42
34	v	201	HEC	CHA-C4D-ND	2.91	127.55	124.42
22	b	603	CLA	C3B-C4B-NB	-2.91	107.94	110.53
22	d	404	CLA	CHB-C4A-NA	2.90	128.59	124.40
29	c	515	DGD	O3G-C3G-C2G	-2.90	103.75	110.82
30	b	618	BCR	C8-C7-C6	-2.90	119.24	127.00
28	D	413	LHG	O3-P-O5	-2.90	97.44	108.94
27	D	409	SQD	C1-C2-C3	-2.90	103.91	110.01
28	d	409	LHG	C26-C25-C24	2.89	123.76	113.13
27	B	621	SQD	O9-S-O7	-2.89	104.41	113.82
22	b	603	CLA	CHD-C1D-ND	-2.89	120.73	124.80
22	C	511	CLA	CAC-C3C-C4C	2.89	128.55	124.79
22	B	610	CLA	CMB-C2B-C3B	2.88	133.33	126.55
30	k	103	BCR	C1-C6-C5	-2.88	118.70	122.64
29	C	516	DGD	O3G-C3G-C2G	-2.88	103.81	110.82
30	C	514	BCR	C15-C14-C13	-2.88	123.24	127.28
28	D	410	LHG	C11-C10-C9	-2.87	99.84	114.37
27	L	101	SQD	C3-C4-C5	2.87	115.44	110.23
22	b	601	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
22	b	606	CLA	CHB-C1B-NB	2.87	128.35	124.05
29	H	103	DGD	O2G-C1B-O1B	-2.87	117.00	123.70
27	f	102	SQD	O5-C1-O6	2.87	116.82	110.04
34	V	201	HEC	CHA-C4D-ND	2.87	127.51	124.42
22	d	405	CLA	CED-O2D-CGD	2.87	122.42	115.92
22	b	601	CLA	C3B-C4B-NB	-2.87	107.97	110.53
29	C	516	DGD	O3E-C3E-C2E	-2.87	103.62	110.38
22	b	604	CLA	C6-C7-C8	-2.87	106.44	115.97
22	B	612	CLA	C4-C3-C5	2.86	120.20	115.23
26	b	622	LMG	O6-C5-C6	2.86	113.53	106.44
29	H	103	DGD	C4E-C3E-C2E	-2.86	105.81	110.83
22	B	615	CLA	C2A-C3A-C4A	2.85	106.48	101.87
22	c	511	CLA	C4-C3-C5	2.85	120.18	115.23
30	k	101	BCR	C11-C10-C9	-2.85	123.28	127.28
23	D	401	PHO	CMA-C3A-C4A	-2.85	108.47	114.61
30	c	514	BCR	C33-C5-C6	-2.85	121.38	124.48
22	B	603	CLA	C6-C7-C8	-2.85	106.50	115.97
27	A	410	SQD	O5-C1-O6	2.84	116.76	110.04
22	c	510	CLA	C16-C15-C13	-2.84	106.53	115.97
23	D	401	PHO	CMB-C2B-C3B	2.84	130.35	124.68
22	b	611	CLA	CAA-C2A-C1A	-2.83	102.70	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404	PHO	CAC-C3C-C2C	2.83	132.75	127.56
22	C	505	CLA	C1-O2A-CGA	-2.82	109.81	116.65
22	a	402	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
22	c	505	CLA	C3B-C4B-NB	-2.82	108.02	110.53
22	b	615	CLA	CMB-C2B-C1B	-2.81	121.14	125.42
27	L	101	SQD	O9-S-O7	-2.81	104.68	113.82
26	c	521	LMG	C1-C2-C3	2.81	115.92	110.01
30	H	102	BCR	C27-C26-C25	2.80	126.49	122.70
22	C	503	CLA	CHC-C4B-NB	2.80	128.25	124.05
30	a	406	BCR	C7-C8-C9	-2.80	122.09	126.23
26	c	520	LMG	O7-C10-O9	-2.80	117.16	123.70
34	f	101	HEC	C1D-ND-C4D	2.80	108.52	105.21
29	c	515	DGD	O2D-C2D-C1D	-2.80	103.41	110.08
22	b	610	CLA	CAA-CBA-CGA	-2.79	105.27	113.21
30	B	618	BCR	C30-C25-C26	-2.79	118.82	122.64
22	B	615	CLA	CHC-C4B-NB	2.79	128.24	124.05
29	H	103	DGD	O6D-C1D-O3G	-2.79	103.45	110.04
22	B	609	CLA	C1-C2-C3	-2.79	121.62	126.20
22	c	512	CLA	O1D-CGD-CBD	2.79	130.02	124.52
30	D	406	BCR	C24-C23-C22	-2.79	122.11	126.23
26	A	409	LMG	C9-C8-C7	-2.79	105.28	111.78
22	c	505	CLA	C4A-NA-C1A	2.79	107.95	106.68
22	C	513	CLA	C3B-C4B-NB	-2.79	108.04	110.53
30	k	103	BCR	C27-C26-C25	2.79	126.47	122.70
29	C	516	DGD	CDB-CCB-CBB	-2.79	100.29	114.37
29	h	101	DGD	O1G-C1A-O1A	-2.79	116.66	123.63
30	a	406	BCR	C38-C26-C27	-2.78	107.66	113.60
22	A	402	CLA	C16-C15-C13	-2.78	106.72	115.97
22	C	506	CLA	CHB-C4A-NA	2.78	128.41	124.40
22	C	504	CLA	CMB-C2B-C1B	-2.78	121.19	125.42
22	B	607	CLA	O2D-CGD-CBD	2.78	116.09	111.23
22	b	608	CLA	CHD-C1D-ND	-2.78	120.89	124.80
30	b	619	BCR	C1-C6-C5	-2.77	118.85	122.64
30	B	616	BCR	C15-C16-C17	-2.77	117.85	123.52
27	B	621	SQD	C4-C3-C2	2.77	115.69	110.83
25	D	407	PL9	C12-C13-C14	-2.77	121.28	127.62
34	f	101	HEC	CMD-C2D-C1D	2.77	129.36	125.03
25	a	409	PL9	C12-C13-C14	-2.77	121.29	127.62
22	B	605	CLA	CHB-C4A-NA	2.76	128.39	124.40
30	I	101	BCR	C38-C26-C27	-2.76	107.71	113.60
30	D	406	BCR	C3-C4-C5	-2.76	109.13	114.06
25	D	407	PL9	C7-C8-C9	-2.76	122.08	126.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	507	CLA	CHD-C1D-ND	-2.76	120.92	124.80
22	A	402	CLA	CMD-C2D-C1D	2.76	129.58	124.73
22	a	405	CLA	CMA-C3A-C4A	-2.76	104.36	111.77
25	a	409	PL9	C30-C29-C28	-2.75	116.56	123.63
26	Y	101	LMG	O2-C2-C1	-2.75	103.52	110.08
22	b	604	CLA	C1-O2A-CGA	-2.75	109.99	116.65
27	L	101	SQD	O47-C7-O49	-2.75	117.28	123.70
22	B	608	CLA	CHD-C4C-NC	2.75	128.49	124.23
22	c	502	CLA	CHD-C1D-ND	-2.74	120.94	124.80
22	b	612	CLA	C3B-C4B-NB	-2.74	108.08	110.53
22	B	611	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
26	D	408	LMG	O2-C2-C1	-2.74	103.56	110.08
22	B	607	CLA	CHD-C1D-ND	-2.74	120.95	124.80
22	B	602	CLA	O1D-CGD-CBD	2.73	129.91	124.52
30	C	514	BCR	C35-C13-C14	-2.73	118.39	122.82
22	B	604	CLA	C16-C15-C13	-2.73	106.89	115.97
22	b	615	CLA	CAA-CBA-CGA	-2.73	105.45	113.21
30	C	515	BCR	C40-C30-C25	2.73	114.52	110.24
34	f	101	HEC	CAC-C3C-C4C	-2.73	121.16	124.91
30	a	406	BCR	C2-C1-C6	2.73	114.40	110.44
26	c	521	LMG	O8-C28-O10	-2.73	116.81	123.63
30	k	101	BCR	C33-C5-C6	-2.73	121.51	124.48
30	x	101	BCR	C38-C26-C25	-2.72	121.51	124.48
22	A	403	CLA	O2D-CGD-CBD	2.72	115.99	111.23
30	d	406	BCR	C16-C15-C14	-2.72	117.94	123.52
29	C	516	DGD	O5D-C6D-C5D	-2.72	103.28	109.42
27	a	410	SQD	O48-C23-C24	2.72	120.14	111.83
26	D	408	LMG	O8-C28-O10	-2.72	116.82	123.63
26	D	408	LMG	O4-C4-C5	2.72	116.03	109.32
26	c	520	LMG	O2-C2-C1	-2.72	103.59	110.08
22	B	602	CLA	C3B-C4B-NB	-2.72	108.10	110.53
23	a	404	PHO	O2D-CGD-O1D	-2.72	118.55	123.85
30	b	619	BCR	C16-C15-C14	-2.72	117.96	123.52
30	b	619	BCR	C12-C13-C14	-2.72	114.74	119.01
22	C	508	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
22	b	613	CLA	CBC-CAC-C3C	2.71	119.78	112.42
22	c	512	CLA	O2A-CGA-O1A	-2.71	116.84	123.63
23	d	401	PHO	C1-C2-C3	-2.71	121.75	126.20
25	A	408	PL9	O2-C1-C6	2.71	124.80	120.48
26	b	622	LMG	C3-C4-C5	-2.71	105.31	110.23
28	d	409	LHG	O8-C23-C24	2.71	120.10	111.83
22	d	403	CLA	CHD-C1D-ND	-2.71	120.99	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	404	CLA	C2D-C1D-ND	-2.71	107.44	110.13
26	a	414	LMG	O6-C5-C4	2.71	114.58	109.70
22	a	403	CLA	C1D-ND-C4D	2.70	108.21	106.31
22	d	404	CLA	CHC-C4B-NB	2.70	128.10	124.05
29	c	516	DGD	CBB-CAB-C9B	-2.70	100.73	114.37
34	V	201	HEC	CMC-C2C-C1C	-2.70	121.31	125.42
22	b	609	CLA	CHB-C4A-NA	2.70	128.29	124.40
30	H	102	BCR	C16-C15-C14	-2.69	118.01	123.52
22	C	503	CLA	CHD-C1D-ND	-2.69	121.01	124.80
22	B	603	CLA	CMB-C2B-C1B	-2.69	121.33	125.42
30	C	514	BCR	C36-C18-C17	-2.69	118.46	122.82
22	C	508	CLA	CHD-C1D-C2D	2.69	131.07	125.49
22	c	508	CLA	CHB-C4A-NA	2.68	128.27	124.40
22	B	611	CLA	O1D-CGD-CBD	2.68	129.81	124.52
22	c	502	CLA	O1D-CGD-CBD	2.68	129.80	124.52
22	d	404	CLA	C2C-C1C-NC	2.68	112.80	109.98
26	c	520	LMG	O6-C1-O1	-2.68	103.72	110.04
22	B	605	CLA	CHD-C4C-NC	2.67	128.38	124.23
22	B	601	CLA	C1-C2-C3	-2.67	121.81	126.20
25	A	408	PL9	O2-C1-C2	-2.67	115.75	121.83
30	x	101	BCR	C35-C13-C14	-2.67	118.48	122.82
30	C	515	BCR	C15-C16-C17	-2.67	118.05	123.52
22	c	505	CLA	CHD-C1D-ND	-2.67	121.04	124.80
22	A	403	CLA	CAC-C3C-C4C	2.67	128.26	124.79
30	c	514	BCR	C29-C30-C25	2.67	114.32	110.44
22	D	405	CLA	O1D-CGD-CBD	2.67	129.78	124.52
31	x	102	STE	O2-C1-C2	2.66	122.42	114.00
23	d	401	PHO	O2A-CGA-O1A	-2.66	116.97	123.63
23	A	404	PHO	OBD-CAD-CBD	-2.66	121.92	125.82
29	A	413	DGD	O6D-C1D-O3G	-2.66	103.75	110.04
22	C	512	CLA	CHD-C1D-ND	-2.66	121.06	124.80
22	b	601	CLA	CHD-C1D-ND	-2.66	121.06	124.80
22	b	605	CLA	CHD-C4C-NC	2.66	128.35	124.23
29	h	101	DGD	C1D-C2D-C3D	-2.66	104.42	110.01
22	B	608	CLA	CBC-CAC-C3C	-2.65	105.22	112.42
26	a	414	LMG	O7-C10-C11	2.65	117.22	111.48
22	B	613	CLA	C2C-C1C-NC	2.65	112.77	109.98
33	D	402	BCT	O3-C-O1	-2.65	112.89	119.68
34	v	201	HEC	CMC-C2C-C1C	-2.65	121.38	125.42
30	D	406	BCR	C27-C26-C25	2.65	126.29	122.70
22	b	608	CLA	CHD-C4C-C3C	-2.65	120.91	124.77
30	x	101	BCR	C2-C1-C6	2.65	114.29	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	605	CLA	C6-C5-C3	-2.64	107.03	113.47
22	c	506	CLA	CHD-C1D-C2D	2.64	130.99	125.49
22	A	402	CLA	O2A-CGA-O1A	-2.64	117.01	123.63
22	a	402	CLA	CHB-C4A-NA	2.64	128.22	124.40
30	b	618	BCR	C15-C16-C17	-2.64	118.11	123.52
30	k	102	BCR	C38-C26-C25	-2.64	121.60	124.48
29	C	516	DGD	O2D-C2D-C1D	-2.64	103.78	110.08
23	a	404	PHO	CMD-C2D-C3D	2.64	129.96	124.68
30	c	514	BCR	C32-C1-C6	-2.64	106.11	110.24
26	B	620	LMG	O7-C10-O9	-2.64	116.55	123.33
22	c	508	CLA	CMD-C2D-C1D	2.64	129.37	124.73
22	c	503	CLA	CHD-C1D-ND	-2.64	121.09	124.80
27	D	409	SQD	C46-C45-C44	-2.63	105.16	113.67
25	a	409	PL9	C32-C33-C34	-2.63	121.59	127.62
22	c	505	CLA	CHB-C4A-NA	2.63	128.20	124.40
29	c	515	DGD	C4E-C3E-C2E	-2.63	106.21	110.83
34	V	201	HEC	C1D-C2D-C3D	-2.63	104.21	106.98
27	A	412	SQD	O47-C45-C46	2.63	112.27	106.21
22	a	402	CLA	C2A-C1A-CHA	2.63	128.43	123.87
22	c	507	CLA	C2C-C1C-NC	2.63	112.74	109.98
30	B	617	BCR	C35-C13-C14	-2.63	118.56	122.82
30	b	617	BCR	C15-C16-C17	-2.63	118.15	123.52
22	C	504	CLA	C4-C3-C5	2.62	119.78	115.23
22	b	605	CLA	C4-C3-C5	2.62	119.78	115.23
22	c	502	CLA	CHB-C1B-NB	2.62	127.98	124.05
22	b	604	CLA	C11-C12-C13	-2.62	107.26	115.97
26	c	521	LMG	O3-C3-C2	-2.62	104.21	110.38
26	d	410	LMG	O1-C1-C2	-2.62	104.30	108.27
22	b	613	CLA	CMB-C2B-C1B	-2.61	121.44	125.42
30	I	101	BCR	C8-C7-C6	-2.61	120.02	127.00
22	b	612	CLA	C1-C2-C3	-2.61	121.92	126.20
22	B	608	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
22	c	503	CLA	C7-C6-C5	-2.61	106.30	113.26
28	D	410	LHG	O8-C23-C24	2.61	119.79	111.83
30	c	514	BCR	C15-C14-C13	-2.61	123.62	127.28
22	C	503	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
30	H	102	BCR	C29-C30-C25	2.60	114.22	110.44
22	b	612	CLA	C11-C12-C13	-2.60	107.33	115.97
34	F	101	HEC	CHD-C1D-ND	2.60	127.58	124.37
22	b	606	CLA	O1D-CGD-CBD	2.60	129.64	124.52
22	D	404	CLA	CHB-C4A-NA	2.59	128.14	124.40
22	D	404	CLA	C16-C15-C13	-2.59	107.35	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	t	101	BCR	C2-C1-C6	2.59	114.20	110.44
30	K	101	BCR	C34-C9-C8	-2.59	114.13	118.09
22	c	511	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
25	D	407	PL9	C42-C43-C44	-2.59	121.70	127.62
22	C	513	CLA	CHB-C4A-NA	2.59	128.13	124.40
22	H	101	CLA	C3B-C4B-NB	-2.59	108.22	110.53
22	C	504	CLA	O2D-CGD-CBD	2.58	115.74	111.23
22	a	402	CLA	O2A-CGA-O1A	-2.58	117.17	123.63
22	C	502	CLA	CHA-C1A-NA	-2.58	120.55	126.39
22	d	403	CLA	CMB-C2B-C1B	-2.58	121.49	125.42
22	b	609	CLA	C7-C6-C5	-2.58	106.39	113.26
26	a	414	LMG	C1-C2-C3	-2.58	104.59	110.01
25	D	407	PL9	C45-C44-C43	-2.58	117.01	123.63
22	a	403	CLA	O2D-CGD-CBD	2.57	115.73	111.23
26	c	520	LMG	O3-C3-C2	-2.57	104.31	110.38
22	b	604	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
22	C	509	CLA	O2D-CGD-CBD	2.57	115.72	111.23
29	h	101	DGD	O3G-C3G-C2G	-2.57	104.57	110.82
22	A	405	CLA	O2A-CGA-O1A	-2.57	117.20	123.63
27	A	410	SQD	O48-C23-O10	-2.57	117.21	123.63
22	C	503	CLA	C4D-CHA-C1A	2.57	124.30	121.24
22	C	501	CLA	CED-O2D-CGD	-2.57	110.10	115.92
26	c	518	LMG	O2-C2-C3	-2.56	104.33	110.38
22	B	607	CLA	C3B-C4B-NB	-2.56	108.24	110.53
22	c	505	CLA	O2A-CGA-O1A	-2.56	117.22	123.63
30	a	406	BCR	C37-C22-C21	-2.56	118.67	122.82
34	V	201	HEC	CHB-C1B-C2B	2.56	129.07	125.03
34	V	201	HEC	C2B-C1B-NB	-2.56	106.94	109.90
22	C	505	CLA	O2A-CGA-O1A	-2.56	117.23	123.63
29	h	101	DGD	O6D-C1D-O3G	-2.55	104.01	110.04
22	B	609	CLA	O1D-CGD-CBD	2.55	129.55	124.52
22	B	611	CLA	CHB-C4A-NA	2.55	128.08	124.40
22	c	508	CLA	C7-C6-C5	-2.55	106.47	113.26
22	b	605	CLA	CHD-C4C-C3C	-2.55	121.06	124.77
29	c	516	DGD	O5D-C6D-C5D	-2.55	103.68	109.42
22	c	503	CLA	C4D-CHA-C1A	2.55	124.28	121.24
22	B	615	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
22	c	503	CLA	CBC-CAC-C3C	-2.54	105.52	112.42
30	a	406	BCR	C20-C21-C22	-2.54	123.71	127.28
22	b	608	CLA	CMA-C3A-C4A	-2.54	104.94	111.77
26	M	101	LMG	C3-C4-C5	-2.54	105.62	110.23
30	K	101	BCR	C35-C13-C14	-2.54	118.70	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	613	CLA	O2D-CGD-CBD	2.54	115.67	111.23
22	B	603	CLA	O1D-CGD-CBD	2.54	129.53	124.52
30	b	619	BCR	C31-C1-C6	2.54	114.22	110.24
22	c	503	CLA	O1D-CGD-CBD	2.54	129.52	124.52
22	B	608	CLA	CHA-C1A-NA	-2.53	120.65	126.39
22	C	513	CLA	CBC-CAC-C3C	2.53	119.29	112.42
22	C	513	CLA	CHC-C1C-NC	2.53	128.13	124.31
30	t	101	BCR	C15-C16-C17	-2.53	118.34	123.52
22	D	405	CLA	CHC-C4B-NB	2.53	127.84	124.05
34	f	101	HEC	CHB-C1B-NB	2.52	127.14	124.42
22	C	505	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
23	A	404	PHO	C4B-NB-C1B	2.52	112.49	108.82
30	K	102	BCR	C1-C6-C5	-2.52	119.20	122.64
30	c	514	BCR	C34-C9-C10	-2.52	118.74	122.82
22	A	403	CLA	CHA-C1A-NA	-2.52	120.69	126.39
22	B	613	CLA	CBC-CAC-C3C	-2.52	105.60	112.42
22	a	405	CLA	C2C-C1C-NC	2.52	112.62	109.98
29	c	515	DGD	C2G-O2G-C1B	2.52	123.82	117.80
30	k	102	BCR	C27-C26-C25	2.52	126.10	122.70
22	b	616	CLA	C6-C5-C3	2.51	119.59	113.47
22	B	608	CLA	C2A-C3A-C4A	2.51	105.93	101.87
30	d	406	BCR	C30-C25-C26	-2.51	119.20	122.64
22	c	501	CLA	O1D-CGD-CBD	2.51	129.47	124.52
22	B	606	CLA	CHD-C1D-ND	-2.51	121.27	124.80
34	F	101	HEC	CAC-C3C-C2C	-2.51	122.92	126.89
25	d	407	PL9	C32-C33-C34	-2.51	121.88	127.62
22	B	604	CLA	CAA-CBA-CGA	-2.51	106.08	113.21
22	B	605	CLA	C2A-C3A-C4A	2.51	105.92	101.87
22	B	602	CLA	CHB-C4A-NA	2.51	128.02	124.40
30	x	101	BCR	C33-C5-C6	-2.51	121.75	124.48
29	C	518	DGD	O3E-C3E-C2E	-2.50	104.47	110.38
27	B	621	SQD	O5-C5-C4	2.50	114.21	109.70
22	A	403	CLA	CED-O2D-CGD	-2.50	110.23	115.92
30	c	514	BCR	C36-C18-C17	-2.50	118.76	122.82
31	R	101	STE	O2-C1-C2	2.50	121.91	114.00
25	a	409	PL9	C7-C8-C9	-2.50	122.52	126.83
29	c	516	DGD	O6E-C1E-O5D	-2.50	104.13	110.04
22	c	513	CLA	O1D-CGD-CBD	2.50	129.45	124.52
30	B	618	BCR	C11-C10-C9	-2.50	123.77	127.28
28	d	409	LHG	O8-C23-O10	-2.50	117.38	123.63
22	D	403	CLA	C11-C12-C13	-2.50	107.66	115.97
23	a	404	PHO	CAC-C3C-C2C	2.50	132.15	127.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	405	CLA	CHA-C1A-NA	-2.50	120.74	126.39
22	C	504	CLA	CED-O2D-CGD	2.49	121.57	115.92
22	b	602	CLA	C2D-C1D-ND	-2.49	107.66	110.13
25	a	409	PL9	C42-C43-C44	-2.49	121.92	127.62
29	c	517	DGD	CDB-CCB-CBB	-2.49	101.77	114.37
26	c	521	LMG	O2-C2-C1	-2.49	104.14	110.08
22	C	502	CLA	CHC-C4B-NB	2.49	127.78	124.05
22	C	512	CLA	C3B-C4B-NB	-2.49	108.31	110.53
29	C	516	DGD	C6D-O5D-C1E	2.49	119.13	113.80
22	b	611	CLA	CAC-C3C-C4C	2.49	128.03	124.79
22	b	603	CLA	CHD-C1D-C2D	2.49	130.66	125.49
34	F	101	HEC	C3C-C4C-NC	-2.49	107.39	110.15
34	f	101	HEC	CHA-C4D-ND	2.49	127.10	124.42
29	A	413	DGD	O5D-C1E-C2E	2.49	112.05	108.27
30	x	101	BCR	C15-C16-C17	-2.48	118.44	123.52
22	b	609	CLA	CMB-C2B-C1B	-2.48	121.64	125.42
22	a	403	CLA	C2D-C1D-ND	-2.48	107.67	110.13
29	c	515	DGD	C3G-C2G-C1G	-2.48	106.01	111.78
22	b	605	CLA	C1D-ND-C4D	-2.48	104.58	106.31
34	v	201	HEC	CHB-C1B-NB	2.47	127.08	124.42
22	b	616	CLA	CHC-C4B-NB	2.47	127.76	124.05
22	b	609	CLA	C6-C5-C3	2.47	119.49	113.47
29	C	517	DGD	O2D-C2D-C1D	-2.47	104.19	110.08
22	c	502	CLA	C1-C2-C3	-2.47	122.15	126.20
30	K	102	BCR	C16-C15-C14	-2.47	118.47	123.52
28	L	102	LHG	C5-O7-C7	-2.47	111.89	117.80
22	C	512	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
26	d	410	LMG	O6-C5-C4	2.47	114.14	109.70
30	B	616	BCR	C29-C30-C25	2.47	114.02	110.44
22	b	601	CLA	O2D-CGD-CBD	2.47	115.54	111.23
26	a	414	LMG	C6-C5-C4	-2.47	106.96	113.02
30	B	616	BCR	C11-C10-C9	-2.47	123.82	127.28
25	D	407	PL9	C8-C7-C3	2.47	118.40	112.03
30	K	101	BCR	C36-C18-C17	-2.46	118.82	122.82
25	A	408	PL9	C11-C9-C8	-2.46	115.64	121.17
22	b	611	CLA	CMD-C2D-C1D	2.46	129.06	124.73
30	b	619	BCR	C7-C8-C9	-2.46	122.59	126.23
22	C	502	CLA	C3B-C4B-NB	-2.46	108.33	110.53
22	d	404	CLA	C1-C2-C3	-2.46	122.17	126.20
30	d	406	BCR	C11-C10-C9	-2.46	123.83	127.28
22	B	608	CLA	C6-C5-C3	2.46	119.45	113.47
30	K	101	BCR	C40-C30-C25	2.45	114.09	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	J	101	STE	O2-C1-C2	2.45	121.75	114.00
22	c	502	CLA	CHB-C1B-C2B	-2.45	120.31	127.43
22	C	503	CLA	C3A-C2A-C1A	2.45	105.01	101.34
30	B	616	BCR	C37-C22-C23	2.45	121.83	118.09
22	C	505	CLA	C4A-NA-C1A	2.45	107.80	106.68
30	C	514	BCR	C29-C30-C25	2.45	114.00	110.44
26	c	520	LMG	O8-C28-O10	-2.45	117.50	123.63
22	C	502	CLA	C2A-C1A-CHA	2.45	128.12	123.87
22	B	602	CLA	C4A-NA-C1A	2.45	107.80	106.68
30	b	618	BCR	C15-C14-C13	-2.44	123.85	127.28
22	B	609	CLA	C3B-C4B-NB	-2.44	108.35	110.53
30	b	618	BCR	C35-C13-C14	-2.44	118.86	122.82
22	c	507	CLA	C1-C2-C3	-2.44	122.20	126.20
22	b	603	CLA	C1-C2-C3	-2.44	122.20	126.20
22	d	403	CLA	CMD-C2D-C1D	2.44	129.02	124.73
29	A	413	DGD	O3E-C3E-C2E	-2.44	104.63	110.38
34	V	201	HEC	C4B-NB-C1B	2.44	108.09	105.21
22	b	611	CLA	C3A-C2A-C1A	2.44	104.99	101.34
25	d	407	PL9	C27-C28-C29	-2.43	122.05	127.62
30	k	103	BCR	C40-C30-C25	2.43	114.06	110.24
22	B	609	CLA	CHC-C1C-NC	2.43	127.97	124.31
29	C	518	DGD	C3G-C2G-C1G	-2.43	106.11	111.78
26	D	408	LMG	C1-O6-C5	-2.43	108.97	113.72
22	C	503	CLA	CHD-C4C-NC	2.43	128.00	124.23
26	M	101	LMG	C38-C37-C36	-2.43	102.08	114.37
29	A	413	DGD	O5D-C6D-C5D	-2.43	103.94	109.42
22	B	603	CLA	C2D-C1D-ND	-2.43	107.72	110.13
22	b	614	CLA	CHB-C4A-NA	2.43	127.91	124.40
26	A	409	LMG	C3-C4-C5	-2.43	105.83	110.23
30	B	616	BCR	C27-C26-C25	2.43	125.99	122.70
22	B	606	CLA	CED-O2D-CGD	2.43	121.43	115.92
25	D	407	PL9	C25-C24-C26	2.43	119.44	115.23
22	c	513	CLA	CHB-C4A-NA	2.43	127.91	124.40
22	b	601	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
22	a	403	CLA	C2A-C1A-CHA	2.43	128.08	123.87
30	B	617	BCR	C7-C8-C9	-2.43	122.64	126.23
22	b	616	CLA	C3B-C4B-NB	-2.42	108.37	110.53
29	c	517	DGD	C3E-C4E-C5E	-2.42	105.84	110.23
22	C	507	CLA	C3B-C4B-NB	-2.42	108.37	110.53
31	X	101	STE	C11-C10-C9	-2.42	102.13	114.37
28	l	101	LHG	O8-C23-C24	2.42	119.21	111.83
29	C	517	DGD	O3G-C1D-C2D	-2.42	104.60	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	410	SQD	O5-C1-C2	-2.42	105.40	110.37
29	h	101	DGD	C2G-O2G-C1B	2.42	123.58	117.80
26	Y	101	LMG	C3-C4-C5	-2.41	105.86	110.23
30	I	101	BCR	C34-C9-C8	-2.41	114.40	118.09
22	b	612	CLA	C11-C10-C8	-2.41	107.95	115.97
30	k	103	BCR	C29-C30-C25	2.41	113.94	110.44
22	C	506	CLA	C2D-C1D-ND	-2.41	107.74	110.13
22	b	610	CLA	O1D-CGD-CBD	2.41	129.27	124.52
28	b	623	LHG	O8-C23-C24	2.41	119.18	111.83
30	x	101	BCR	C36-C18-C17	-2.41	118.91	122.82
22	C	510	CLA	C1D-ND-C4D	2.41	108.00	106.31
22	C	506	CLA	OBD-CAD-C3D	2.41	134.04	128.42
30	C	514	BCR	C11-C10-C9	-2.40	123.91	127.28
26	d	410	LMG	O2-C2-C1	-2.40	104.35	110.08
22	A	405	CLA	CHB-C4A-NA	2.40	127.86	124.40
22	c	508	CLA	CHD-C1D-C2D	2.40	130.48	125.49
22	c	504	CLA	OBD-CAD-C3D	2.40	134.01	128.42
22	B	603	CLA	C1D-ND-C4D	2.39	107.99	106.31
22	A	402	CLA	CHD-C4C-NC	2.39	127.94	124.23
25	d	407	PL9	C8-C7-C3	2.39	118.22	112.03
23	A	404	PHO	C1A-C2A-C3A	-2.39	100.56	102.84
22	A	402	CLA	C3D-C2D-C1D	-2.39	102.57	105.83
27	A	410	SQD	O8-S-C6	2.39	110.59	105.97
27	D	409	SQD	O9-S-O7	-2.39	106.06	113.82
22	B	602	CLA	C5-C3-C2	-2.38	115.81	121.17
22	d	404	CLA	C16-C15-C13	-2.38	108.04	115.97
22	c	511	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
22	B	612	CLA	C7-C6-C5	-2.38	106.91	113.26
22	A	402	CLA	CHD-C4C-C3C	-2.38	121.30	124.77
34	v	201	HEC	CBA-CAA-C2A	-2.38	105.94	112.53
22	c	502	CLA	CHD-C1D-C2D	2.38	130.44	125.49
28	a	411	LHG	C11-C10-C9	-2.38	102.34	114.37
22	B	604	CLA	CHB-C4A-NA	2.38	127.83	124.40
22	b	601	CLA	CHD-C4C-NC	2.38	127.92	124.23
22	c	502	CLA	CMB-C2B-C3B	2.38	132.14	126.55
30	B	617	BCR	C15-C14-C13	-2.38	123.94	127.28
23	a	404	PHO	O2A-CGA-O1A	-2.38	117.68	123.63
22	c	511	CLA	CMA-C3A-C4A	2.38	118.16	111.77
27	A	412	SQD	O49-C7-C8	-2.38	114.49	123.78
29	c	516	DGD	O5D-C1E-C2E	2.38	111.88	108.27
22	D	403	CLA	CHB-C4A-NA	2.37	127.83	124.40
29	H	103	DGD	CCB-CBB-CAB	-2.37	102.37	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	601	CLA	C2B-C1B-NB	-2.37	107.86	110.33
22	B	614	CLA	CHC-C1C-C2C	-2.37	120.20	126.95
29	C	518	DGD	O1G-C1A-O1A	-2.37	117.69	123.63
29	C	517	DGD	C7B-C6B-C5B	-2.37	102.38	114.37
22	b	608	CLA	C4A-NA-C1A	2.37	107.76	106.68
22	b	605	CLA	C3D-C4D-ND	2.37	113.84	109.99
22	C	512	CLA	O1D-CGD-CBD	2.37	129.19	124.52
30	K	102	BCR	C10-C11-C12	-2.36	116.35	123.20
29	c	516	DGD	O2G-C1B-O1B	-2.36	118.18	123.70
22	B	605	CLA	C3B-C4B-NB	-2.36	108.42	110.53
29	C	517	DGD	C1D-O6D-C5D	-2.36	109.11	113.72
22	b	612	CLA	O2A-CGA-CBA	2.36	119.03	111.83
29	C	518	DGD	O3D-C3D-C4D	-2.36	104.81	110.38
22	A	403	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
30	a	406	BCR	C39-C30-C25	-2.36	106.54	110.24
29	c	516	DGD	CDB-CCB-CBB	-2.36	102.44	114.37
26	c	521	LMG	C4-C3-C2	2.36	114.97	110.83
27	B	621	SQD	O8-S-C6	2.36	110.52	105.97
25	d	407	PL9	C50-C49-C48	-2.36	115.59	122.66
22	B	603	CLA	CMB-C2B-C3B	2.36	132.09	126.55
22	b	611	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
22	c	504	CLA	C4-C3-C5	2.35	119.31	115.23
29	c	515	DGD	O5D-C6D-C5D	-2.35	104.12	109.42
28	A	411	LHG	O8-C23-C24	2.35	119.01	111.83
30	c	514	BCR	C38-C26-C27	-2.35	108.58	113.60
29	C	516	DGD	C5B-C4B-C3B	-2.35	102.49	114.37
22	B	601	CLA	CHB-C4A-NA	2.35	127.79	124.40
30	d	406	BCR	C19-C18-C17	-2.35	115.32	119.01
22	d	403	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
30	T	101	BCR	C3-C4-C5	-2.34	109.88	114.06
25	D	407	PL9	C7-C3-C2	-2.34	120.63	123.39
30	B	617	BCR	C2-C1-C6	2.34	113.84	110.44
29	A	413	DGD	O3D-C3D-C4D	-2.34	104.86	110.38
22	C	509	CLA	CHA-C1A-NA	-2.34	121.10	126.39
26	c	518	LMG	O8-C28-O10	-2.34	117.78	123.63
22	c	511	CLA	O1A-CGA-CBA	2.34	132.92	123.78
22	b	610	CLA	C2C-C1C-NC	2.34	112.44	109.98
22	b	612	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
22	b	602	CLA	C3B-C4B-NB	-2.33	108.45	110.53
30	C	515	BCR	C27-C26-C25	2.33	125.85	122.70
22	c	504	CLA	C6-C7-C8	-2.33	108.23	115.97
22	B	601	CLA	C4A-NA-C1A	2.32	107.74	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	x	101	BCR	C7-C8-C9	-2.32	122.80	126.23
25	A	408	PL9	C40-C39-C38	-2.32	117.67	123.63
34	f	101	HEC	CHD-C4C-NC	2.32	128.07	123.86
27	D	409	SQD	C3-C4-C5	2.32	114.44	110.23
29	h	101	DGD	C1E-O6E-C5E	2.32	118.25	113.72
30	b	617	BCR	C34-C9-C10	-2.32	119.06	122.82
22	B	603	CLA	O2A-CGA-CBA	2.32	118.90	111.83
25	a	409	PL9	C20-C19-C21	2.32	119.25	115.23
34	V	201	HEC	CBD-CAD-C3D	-2.32	106.13	112.53
22	C	504	CLA	C2C-C1C-NC	2.31	112.41	109.98
22	a	402	CLA	C4-C3-C5	2.31	119.24	115.23
22	b	603	CLA	CHB-C1B-C2B	-2.31	120.71	127.43
26	M	101	LMG	O5-C6-C5	-2.31	103.46	111.33
22	b	609	CLA	CHA-C1A-NA	-2.31	121.15	126.39
26	c	520	LMG	O1-C1-C2	-2.31	104.76	108.27
29	h	101	DGD	O3E-C3E-C2E	-2.31	104.93	110.38
29	H	103	DGD	C6D-C5D-C4D	2.31	116.92	112.07
22	C	509	CLA	CAA-C2A-C3A	-2.31	106.75	113.00
27	B	621	SQD	O49-C7-C8	-2.31	114.75	123.78
29	A	413	DGD	C3E-C4E-C5E	-2.31	106.04	110.23
22	C	508	CLA	C3C-C4C-NC	-2.31	107.47	110.43
22	B	614	CLA	CMC-C2C-C3C	2.31	132.39	126.15
30	b	618	BCR	C28-C27-C26	-2.31	109.94	114.06
25	a	409	PL9	O2-C1-C2	-2.31	116.58	121.83
27	a	410	SQD	O5-C5-C4	2.30	113.85	109.70
22	b	611	CLA	CHB-C4A-NA	2.30	127.72	124.40
22	C	508	CLA	CHB-C1B-NB	2.30	127.50	124.05
30	K	102	BCR	C12-C13-C14	-2.30	115.39	119.01
23	d	401	PHO	C4B-NB-C1B	2.30	112.17	108.82
22	b	614	CLA	O2D-CGD-CBD	2.30	115.25	111.23
27	L	101	SQD	O8-S-C6	2.30	110.41	105.97
22	b	602	CLA	C1-C2-C3	-2.30	122.43	126.20
29	C	517	DGD	CDB-CCB-CBB	-2.30	102.75	114.37
22	c	504	CLA	CED-O2D-CGD	2.30	121.12	115.92
30	K	102	BCR	C39-C30-C25	-2.30	106.64	110.24
22	A	405	CLA	C4-C3-C5	2.29	119.21	115.23
22	B	605	CLA	CHD-C4C-C3C	-2.29	121.43	124.77
22	B	604	CLA	CMC-C2C-C1C	2.29	128.62	125.03
22	B	605	CLA	CHD-C1D-ND	-2.29	121.58	124.80
30	K	102	BCR	C30-C25-C26	-2.29	119.50	122.64
28	D	411	LHG	O8-C23-C24	2.29	118.83	111.83
30	C	515	BCR	C2-C1-C6	2.29	113.77	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	601	CLA	C6-C5-C3	-2.29	107.89	113.47
22	c	506	CLA	CBC-CAC-C3C	-2.29	106.22	112.42
22	a	405	CLA	C4D-CHA-C1A	-2.29	118.51	121.24
22	C	508	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
26	D	412	LMG	C38-C37-C36	-2.29	102.80	114.37
22	C	508	CLA	C7-C6-C5	-2.29	107.16	113.26
30	c	514	BCR	C11-C10-C9	-2.29	124.07	127.28
22	b	607	CLA	CBC-CAC-C3C	-2.29	106.22	112.42
22	c	510	CLA	C6-C5-C3	-2.29	107.90	113.47
22	C	513	CLA	CHD-C1D-ND	-2.29	121.59	124.80
22	C	508	CLA	O1D-CGD-CBD	2.29	129.03	124.52
22	b	607	CLA	CHD-C1D-ND	-2.28	121.59	124.80
22	c	505	CLA	CHA-C1A-NA	-2.28	121.22	126.39
22	c	504	CLA	O2D-CGD-O1D	-2.28	119.40	123.85
22	B	615	CLA	O1D-CGD-CBD	2.28	129.02	124.52
27	a	410	SQD	O5-C1-O6	2.28	115.44	110.04
26	M	101	LMG	O7-C10-O9	-2.28	118.37	123.70
22	C	501	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
22	B	607	CLA	CHB-C1B-NB	2.28	127.47	124.05
22	B	613	CLA	C1C-C2C-C3C	-2.28	104.58	106.98
30	T	101	BCR	C38-C26-C27	-2.28	108.73	113.60
22	B	614	CLA	CMC-C2C-C1C	-2.28	121.47	125.03
22	a	405	CLA	C1C-C2C-C3C	-2.28	104.59	106.98
26	c	518	LMG	O7-C10-O9	-2.28	118.60	122.99
30	I	101	BCR	C16-C17-C18	-2.27	124.09	127.28
22	b	602	CLA	C4-C3-C5	2.27	119.17	115.23
26	c	521	LMG	O2-C2-C3	-2.27	105.02	110.38
22	b	611	CLA	CAA-CBA-CGA	-2.27	106.76	113.21
27	D	409	SQD	O48-C23-O10	-2.27	117.95	123.63
28	D	411	LHG	O8-C23-O10	-2.27	117.95	123.63
30	B	617	BCR	C40-C30-C29	-2.27	100.23	108.95
23	a	404	PHO	C1-C2-C3	-2.27	122.48	126.20
22	c	510	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
30	t	101	BCR	C29-C30-C25	2.27	113.73	110.44
22	b	603	CLA	OBD-CAD-C3D	2.27	133.72	128.42
22	b	605	CLA	C4D-C3D-CAD	-2.27	105.64	108.11
22	c	501	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
22	c	502	CLA	C4D-C3D-CAD	-2.26	105.65	108.11
31	X	101	STE	C3-C2-C1	-2.26	108.60	114.51
22	d	405	CLA	O1D-CGD-CBD	2.26	128.98	124.52
22	d	404	CLA	C2A-C1A-CHA	2.26	127.79	123.87
27	a	410	SQD	O47-C7-C8	2.26	116.37	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	606	CLA	C1C-C2C-C3C	-2.26	104.61	106.98
26	A	409	LMG	O3-C3-C2	-2.26	105.06	110.38
23	A	404	PHO	CMB-C2B-C3B	2.26	129.19	124.68
22	c	504	CLA	O2D-CGD-CBD	2.25	115.17	111.23
22	b	604	CLA	C4D-C3D-CAD	-2.25	105.66	108.11
27	L	101	SQD	O48-C23-O10	-2.25	117.99	123.63
22	C	502	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
22	B	603	CLA	C2A-C1A-CHA	2.25	127.78	123.87
26	a	414	LMG	C9-C8-C7	-2.25	106.53	111.78
22	c	504	CLA	C3D-C4D-ND	2.25	113.65	109.99
22	B	603	CLA	C3B-C4B-NB	-2.25	108.52	110.53
22	C	506	CLA	CGD-CBD-CAD	-2.25	103.56	110.85
30	B	618	BCR	C27-C26-C25	2.25	125.74	122.70
26	Y	101	LMG	O6-C5-C6	2.25	112.01	106.44
26	c	520	LMG	C9-C8-C7	-2.25	106.54	111.78
29	c	516	DGD	C7B-C6B-C5B	-2.25	103.00	114.37
22	c	513	CLA	CHD-C1D-ND	-2.25	121.64	124.80
25	A	408	PL9	C27-C28-C29	-2.25	122.48	127.62
29	A	413	DGD	C3G-C2G-C1G	-2.25	106.55	111.78
22	B	615	CLA	C3B-C4B-NB	-2.25	108.53	110.53
30	I	101	BCR	C15-C16-C17	-2.24	118.93	123.52
22	B	601	CLA	CHA-C4D-ND	2.24	137.18	132.55
26	A	409	LMG	O8-C28-O10	-2.24	118.02	123.63
22	d	403	CLA	C1-C2-C3	-2.24	122.53	126.20
30	B	617	BCR	C15-C16-C17	-2.24	118.94	123.52
27	A	412	SQD	O48-C46-C45	2.24	114.72	108.35
26	A	409	LMG	O5-C6-C5	-2.24	103.72	111.33
30	K	101	BCR	C37-C22-C23	2.24	121.50	118.09
22	C	511	CLA	C4-C3-C5	2.24	119.11	115.23
22	c	511	CLA	O2A-C1-C2	-2.23	99.51	108.11
26	Y	101	LMG	O7-C10-O9	-2.23	118.48	123.70
30	C	515	BCR	C8-C7-C6	-2.23	121.03	127.00
22	B	605	CLA	CHA-C1A-NA	-2.23	121.34	126.39
22	b	615	CLA	CHB-C1B-C2B	-2.23	120.95	127.43
22	C	502	CLA	CMD-C2D-C3D	2.23	132.81	127.69
22	B	601	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
26	Y	101	LMG	O6-C1-O1	-2.23	104.77	110.04
29	h	101	DGD	O6E-C5E-C4E	2.23	113.72	109.70
30	x	101	BCR	C36-C18-C19	2.23	121.49	118.09
26	d	410	LMG	O3-C3-C2	-2.23	105.12	110.38
22	A	405	CLA	CHD-C1D-C2D	2.23	130.12	125.49
22	b	611	CLA	CGD-CBD-CAD	-2.23	103.64	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	d	411	STE	O2-C1-C2	2.23	121.04	114.00
25	d	407	PL9	C20-C19-C21	2.23	119.09	115.23
29	c	516	DGD	O6E-C5E-C4E	2.23	113.71	109.70
29	c	516	DGD	O3D-C3D-C4D	-2.23	105.13	110.38
30	x	101	BCR	C34-C9-C8	-2.22	114.69	118.09
22	a	405	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
29	c	515	DGD	C3D-C4D-C5D	-2.22	106.20	110.23
22	C	511	CLA	C2A-C1A-CHA	2.22	127.72	123.87
22	A	403	CLA	CHB-C4A-NA	2.22	127.61	124.40
22	A	402	CLA	CHC-C1C-NC	2.22	127.66	124.31
22	B	610	CLA	C14-C13-C15	-2.22	103.35	111.27
22	A	405	CLA	CHD-C4C-NC	2.22	127.68	124.23
25	d	407	PL9	C51-C49-C50	2.22	119.70	114.59
25	d	407	PL9	C7-C8-C9	-2.22	123.00	126.83
22	b	604	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
22	b	603	CLA	C7-C6-C5	-2.22	107.35	113.26
30	b	617	BCR	C15-C14-C13	-2.22	124.17	127.28
22	C	508	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
30	k	101	BCR	C27-C26-C25	2.22	125.70	122.70
27	D	409	SQD	C1-O5-C5	-2.22	109.39	113.72
22	D	405	CLA	O2A-CGA-O1A	-2.22	118.09	123.63
34	V	201	HEC	CHC-C1C-NC	2.22	127.88	123.86
30	I	101	BCR	C16-C15-C14	-2.21	118.99	123.52
26	D	412	LMG	O7-C10-O9	-2.21	118.53	123.70
22	B	613	CLA	CHB-C1B-NB	2.21	127.37	124.05
22	c	511	CLA	CHD-C1D-ND	-2.21	121.69	124.80
27	f	102	SQD	O5-C1-C2	-2.21	105.83	110.37
22	C	506	CLA	C1D-ND-C4D	2.21	107.86	106.31
25	A	408	PL9	C25-C24-C23	-2.21	117.95	123.63
23	D	401	PHO	C4B-NB-C1B	2.21	112.04	108.82
23	A	404	PHO	O2D-CGD-O1D	-2.21	119.55	123.85
25	a	409	PL9	O2-C1-C6	2.21	123.99	120.48
22	b	615	CLA	C3A-C2A-C1A	2.21	104.65	101.34
25	d	407	PL9	C40-C39-C38	-2.21	117.96	123.63
22	b	610	CLA	C4-C3-C5	2.21	119.06	115.23
26	B	620	LMG	O8-C28-O10	-2.21	117.66	123.33
31	t	103	STE	C3-C2-C1	-2.21	108.75	114.51
22	B	602	CLA	CHD-C4C-C3C	-2.20	121.56	124.77
22	B	602	CLA	CHC-C1C-NC	2.20	127.63	124.31
22	b	610	CLA	CAC-C3C-C4C	2.20	127.66	124.79
27	t	102	SQD	O49-C7-C8	-2.20	115.17	123.78
22	c	509	CLA	C16-C15-C13	-2.20	108.64	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	514	BCR	C31-C1-C6	-2.20	106.79	110.24
30	t	101	BCR	C1-C6-C5	-2.20	119.63	122.64
30	t	101	BCR	C35-C13-C14	-2.20	119.25	122.82
30	k	101	BCR	C36-C18-C17	-2.20	119.26	122.82
22	b	603	CLA	C1-O2A-CGA	2.20	121.97	116.65
29	c	516	DGD	C9A-C8A-C7A	-2.20	103.27	114.37
30	x	101	BCR	C35-C13-C12	2.19	121.44	118.09
22	b	613	CLA	C3B-C4B-NB	-2.19	108.57	110.53
31	t	103	STE	O2-C1-C2	2.19	120.93	114.00
29	c	515	DGD	C4D-C3D-C2D	-2.19	106.98	110.83
30	B	616	BCR	C8-C7-C6	-2.19	121.14	127.00
30	I	101	BCR	C37-C22-C21	-2.19	119.26	122.82
27	f	102	SQD	C45-O47-C7	2.19	123.04	117.80
22	C	510	CLA	CBC-CAC-C3C	-2.19	106.49	112.42
34	f	101	HEC	CBA-CAA-C2A	-2.19	106.48	112.53
22	B	604	CLA	CHD-C1D-ND	-2.19	121.72	124.80
30	B	618	BCR	C15-C16-C17	-2.19	119.05	123.52
28	D	411	LHG	C18-C17-C16	-2.18	103.32	114.37
22	C	513	CLA	O2D-CGD-CBD	2.18	115.05	111.23
22	B	601	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
25	A	408	PL9	C12-C13-C14	-2.18	122.63	127.62
25	d	407	PL9	C7-C3-C4	2.18	118.71	116.91
22	a	403	CLA	CHA-C1A-NA	-2.18	121.45	126.39
22	c	504	CLA	CHB-C4A-NA	2.18	127.55	124.40
22	a	403	CLA	O2D-CGD-O1D	-2.18	119.60	123.85
28	D	410	LHG	C18-C17-C16	-2.18	103.35	114.37
22	c	502	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
22	B	610	CLA	O1A-CGA-CBA	2.18	132.31	123.78
31	b	621	STE	C3-C2-C1	-2.18	108.82	114.51
22	c	503	CLA	C3B-C4B-NB	-2.18	108.59	110.53
22	c	509	CLA	O2D-CGD-CBD	2.18	115.04	111.23
22	b	606	CLA	CED-O2D-CGD	-2.18	110.98	115.92
27	a	410	SQD	O8-S-O9	-2.18	105.95	111.40
26	a	414	LMG	O7-C10-O9	-2.18	118.62	123.70
22	b	615	CLA	C7-C6-C5	-2.18	107.46	113.26
29	C	516	DGD	CAB-C9B-C8B	-2.18	103.37	114.37
22	b	602	CLA	CHA-C4D-ND	2.18	137.04	132.55
30	t	101	BCR	C33-C5-C6	-2.18	122.11	124.48
29	c	515	DGD	O3D-C3D-C4D	-2.18	105.25	110.38
22	b	613	CLA	CMB-C2B-C3B	2.18	131.67	126.55
30	B	617	BCR	C3-C4-C5	-2.18	110.18	114.06
29	A	413	DGD	C1E-O6E-C5E	2.17	117.97	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	405	CLA	C2D-C1D-ND	-2.17	107.97	110.13
26	A	409	LMG	C1-O6-C5	-2.17	109.47	113.72
22	B	609	CLA	O2D-CGD-CBD	2.17	115.03	111.23
22	A	402	CLA	C3B-C4B-NB	-2.17	108.59	110.53
26	Y	101	LMG	O1-C7-C8	-2.17	105.53	110.82
22	c	501	CLA	CHA-C1A-NA	-2.17	121.47	126.39
22	B	614	CLA	CMD-C2D-C1D	2.17	128.55	124.73
22	C	513	CLA	CHB-C1B-NB	2.17	127.31	124.05
30	a	406	BCR	C29-C30-C25	2.17	113.59	110.44
30	b	619	BCR	C20-C21-C22	-2.17	124.23	127.28
30	b	619	BCR	C37-C22-C21	-2.17	119.30	122.82
30	t	101	BCR	C12-C13-C14	-2.17	115.60	119.01
22	B	614	CLA	CHD-C1D-ND	-2.17	121.75	124.80
34	v	201	HEC	CHC-C1C-NC	2.17	127.79	123.86
22	c	508	CLA	CHD-C4C-NC	2.17	127.59	124.23
25	d	407	PL9	O2-C1-C6	2.17	123.92	120.48
22	c	502	CLA	C1D-ND-C4D	2.16	107.83	106.31
22	C	501	CLA	CHD-C4C-NC	2.16	127.59	124.23
29	A	413	DGD	C1D-C2D-C3D	-2.16	105.46	110.01
22	B	614	CLA	CHC-C1C-NC	2.16	127.57	124.31
22	D	404	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
22	b	609	CLA	C4-C3-C5	-2.16	111.47	115.23
22	b	610	CLA	C3B-C2B-C1B	-2.16	104.62	107.17
22	b	607	CLA	C3A-C2A-C1A	2.16	104.58	101.34
22	b	605	CLA	C3B-C4B-NB	-2.16	108.60	110.53
28	L	102	LHG	C12-C11-C10	-2.16	103.45	114.37
22	c	507	CLA	O1A-CGA-CBA	2.16	132.23	123.78
29	h	101	DGD	C7B-C6B-C5B	-2.16	103.45	114.37
30	b	617	BCR	C11-C10-C9	-2.16	124.25	127.28
30	K	101	BCR	C30-C25-C26	-2.16	119.69	122.64
22	A	402	CLA	C7-C6-C5	-2.16	107.52	113.26
22	d	403	CLA	C3B-C4B-NB	-2.15	108.61	110.53
22	B	602	CLA	CHC-C1C-C2C	-2.15	120.83	126.95
22	c	502	CLA	C4D-CHA-C1A	2.15	123.81	121.24
22	B	614	CLA	C6-C7-C8	-2.15	108.81	115.97
29	C	518	DGD	O2D-C2D-C1D	-2.15	104.95	110.08
22	B	603	CLA	CHA-C1A-NA	-2.15	121.52	126.39
22	c	509	CLA	O1D-CGD-CBD	2.15	128.76	124.52
22	c	509	CLA	C1-O2A-CGA	-2.15	111.45	116.65
22	C	506	CLA	CHA-C1A-NA	-2.15	121.53	126.39
22	B	601	CLA	CGD-CBD-CAD	-2.15	103.89	110.85
22	B	608	CLA	CHB-C4A-NA	2.15	127.50	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	f	101	HEC	CHC-C4B-C3B	2.15	129.19	125.23
30	a	406	BCR	C16-C17-C18	-2.15	124.27	127.28
34	F	101	HEC	C4D-C3D-C2D	-2.15	103.77	106.89
22	B	608	CLA	CHB-C1B-NB	2.14	127.27	124.05
22	b	606	CLA	CHB-C1B-C2B	-2.14	121.20	127.43
34	V	201	HEC	C1C-C2C-C3C	2.14	109.27	106.82
22	d	405	CLA	CMA-C3A-C2A	-2.14	105.69	113.98
22	b	606	CLA	C3C-C4C-NC	-2.14	107.69	110.43
22	B	602	CLA	CHD-C4C-NC	2.14	127.55	124.23
30	C	515	BCR	C10-C11-C12	-2.14	117.00	123.20
34	v	201	HEC	CAB-C3B-C2B	-2.14	123.62	127.56
22	c	507	CLA	C7-C6-C5	-2.14	107.56	113.26
30	B	618	BCR	C1-C6-C5	-2.14	119.71	122.64
22	B	612	CLA	C2A-C1A-CHA	2.14	127.58	123.87
30	b	618	BCR	C11-C10-C9	-2.14	124.28	127.28
28	a	411	LHG	C20-C19-C18	-2.14	103.57	114.37
22	D	403	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
23	A	404	PHO	O2D-CGD-CBD	2.13	113.29	110.95
29	C	517	DGD	C5B-C4B-C3B	-2.13	103.58	114.37
29	A	413	DGD	O5E-C6E-C5E	-2.13	104.06	111.33
22	b	606	CLA	C6-C5-C3	-2.13	108.27	113.47
22	d	405	CLA	CHD-C1D-ND	-2.13	121.80	124.80
23	d	401	PHO	C3B-C4B-NB	-2.13	106.07	107.46
29	C	516	DGD	O1G-C1A-O1A	2.13	128.96	123.63
23	D	401	PHO	CMD-C2D-C3D	2.13	128.94	124.68
22	B	607	CLA	CHD-C4C-NC	2.13	127.53	124.23
26	M	101	LMG	C1-C2-C3	-2.13	105.53	110.01
29	A	413	DGD	CAB-C9B-C8B	-2.13	103.61	114.37
22	C	508	CLA	CHD-C4C-NC	2.13	127.53	124.23
23	a	404	PHO	C4B-NB-C1B	2.13	111.92	108.82
22	c	503	CLA	CMA-C3A-C4A	2.13	117.49	111.77
23	A	404	PHO	CMA-C3A-C4A	-2.13	110.03	114.61
29	h	101	DGD	CBB-CAB-C9B	-2.13	103.62	114.37
22	C	501	CLA	CHB-C1B-NB	2.13	127.24	124.05
22	C	504	CLA	CHA-C1A-NA	-2.13	121.58	126.39
22	C	510	CLA	C11-C10-C8	-2.13	108.90	115.97
27	A	410	SQD	O47-C45-C44	2.13	115.97	108.34
29	C	517	DGD	CAB-C9B-C8B	-2.12	103.63	114.37
22	C	508	CLA	C3B-C4B-NB	-2.12	108.64	110.53
30	t	101	BCR	C27-C26-C25	2.12	125.57	122.70
22	B	608	CLA	C3B-C4B-NB	-2.12	108.64	110.53
27	L	101	SQD	O10-C23-C24	-2.12	115.48	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	603	CLA	C1-C2-C3	-2.12	122.72	126.20
22	D	403	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
22	C	503	CLA	O1D-CGD-CBD	2.12	128.70	124.52
29	A	413	DGD	C4E-C3E-C2E	-2.12	107.11	110.83
29	c	516	DGD	C4E-C3E-C2E	-2.12	107.11	110.83
27	L	101	SQD	O49-C7-C8	-2.12	115.50	123.78
22	B	601	CLA	C1C-C2C-C3C	-2.12	104.75	106.98
26	m	101	LMG	O8-C28-O10	-2.12	118.34	123.63
29	H	103	DGD	CAB-C9B-C8B	-2.12	103.67	114.37
31	C	521	STE	O2-C1-C2	2.12	120.68	114.00
22	B	602	CLA	C4D-C3D-CAD	-2.11	105.81	108.11
30	B	616	BCR	C30-C25-C26	-2.11	119.75	122.64
29	c	517	DGD	C5B-C4B-C3B	-2.11	103.68	114.37
22	b	601	CLA	O2A-CGA-CBA	2.11	118.27	111.83
22	D	404	CLA	C3D-C4D-ND	2.11	113.42	109.99
31	B	625	STE	O2-C1-O1	-2.11	117.90	123.33
30	b	618	BCR	C37-C22-C21	-2.11	119.40	122.82
27	a	410	SQD	O8-S-O7	2.11	116.68	111.40
22	c	506	CLA	C1-O2A-CGA	2.11	121.76	116.65
26	c	521	LMG	O6-C1-O1	-2.11	105.06	110.04
22	H	101	CLA	O2D-CGD-CBD	2.11	114.91	111.23
22	A	405	CLA	C6-C5-C3	2.11	118.60	113.47
22	D	404	CLA	C1C-C2C-C3C	-2.11	104.77	106.98
28	D	411	LHG	O3-P-O5	-2.10	100.59	108.94
29	c	515	DGD	O3E-C3E-C2E	-2.10	105.42	110.38
34	f	101	HEC	C3C-C4C-NC	-2.10	107.82	110.15
30	C	515	BCR	C30-C25-C26	-2.10	119.76	122.64
22	C	513	CLA	CHD-C1D-C2D	2.10	129.86	125.49
31	C	521	STE	C4-C3-C2	-2.10	105.40	113.13
34	F	101	HEC	CHA-C1A-NA	2.10	126.74	124.45
31	M	102	STE	O2-C1-O1	-2.10	117.93	123.33
31	x	102	STE	O2-C1-O1	-2.10	117.93	123.33
22	d	405	CLA	CMB-C2B-C3B	2.10	131.49	126.55
22	c	503	CLA	CHC-C1C-NC	2.10	127.47	124.31
30	a	406	BCR	C30-C25-C26	-2.10	119.77	122.64
28	A	411	LHG	O8-C23-O10	-2.10	118.38	123.63
27	B	621	SQD	O47-C45-C46	2.10	115.87	108.34
28	D	410	LHG	C27-C26-C25	-2.10	103.76	114.37
22	B	613	CLA	C2B-C1B-NB	-2.10	108.15	110.33
26	D	408	LMG	O7-C10-O9	-2.10	118.80	123.70
30	b	619	BCR	C11-C10-C9	-2.09	124.34	127.28
28	D	413	LHG	C11-C10-C9	-2.09	103.78	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	505	CLA	CBA-CAA-C2A	2.09	120.02	113.79
22	A	402	CLA	CBC-CAC-C3C	2.09	118.09	112.42
25	d	407	PL9	O1-C4-C3	-2.09	118.52	120.73
22	H	101	CLA	C2B-C1B-NB	-2.09	108.16	110.33
26	A	409	LMG	C20-C19-C18	-2.09	103.80	114.37
22	b	603	CLA	C4-C3-C5	2.09	118.86	115.23
25	D	407	PL9	C37-C38-C39	-2.09	122.84	127.62
22	c	507	CLA	CHA-C1A-NA	-2.09	121.66	126.39
22	c	508	CLA	CHA-C1A-NA	-2.09	121.66	126.39
30	D	406	BCR	C28-C27-C26	-2.09	110.33	114.06
30	b	617	BCR	C3-C4-C5	-2.09	110.33	114.06
30	b	618	BCR	C16-C15-C14	-2.09	119.25	123.52
30	C	514	BCR	C2-C1-C6	2.09	113.47	110.44
22	C	503	CLA	C1-O2A-CGA	2.09	121.70	116.65
22	b	608	CLA	CHD-C1D-C2D	2.09	129.83	125.49
22	C	509	CLA	CED-O2D-CGD	2.09	120.65	115.92
22	B	607	CLA	CHB-C4A-NA	2.09	127.41	124.40
34	V	201	HEC	CAA-C2A-C1A	2.08	129.09	124.85
22	d	405	CLA	C3B-C4B-NB	-2.08	108.67	110.53
30	d	406	BCR	C7-C8-C9	-2.08	123.15	126.23
30	b	617	BCR	C32-C1-C6	-2.08	106.97	110.24
22	C	510	CLA	C1-O2A-CGA	2.08	121.69	116.65
22	d	405	CLA	CHA-C1A-NA	-2.08	121.67	126.39
22	c	506	CLA	C3C-C4C-NC	-2.08	107.76	110.43
22	c	504	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
29	c	515	DGD	O6E-C1E-O5D	-2.08	105.13	110.04
22	b	604	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
25	a	409	PL9	C22-C23-C24	-2.08	122.86	127.62
22	c	509	CLA	CMB-C2B-C3B	2.08	131.44	126.55
30	H	102	BCR	C38-C26-C25	-2.08	122.21	124.48
30	k	101	BCR	C35-C13-C14	-2.08	119.45	122.82
30	C	514	BCR	C40-C30-C25	2.08	113.50	110.24
26	m	101	LMG	C1-O6-C5	-2.08	109.66	113.72
30	I	101	BCR	C32-C1-C6	2.08	113.50	110.24
22	c	509	CLA	CHC-C1C-C2C	-2.08	121.04	126.95
28	d	408	LHG	C20-C19-C18	-2.08	103.87	114.37
22	B	608	CLA	CHC-C4B-NB	2.08	127.17	124.05
30	k	101	BCR	C20-C21-C22	-2.08	124.36	127.28
30	C	514	BCR	C36-C18-C19	2.08	121.26	118.09
30	K	102	BCR	C8-C9-C10	-2.08	115.74	119.01
29	h	101	DGD	O2E-C2E-C1E	-2.08	105.13	110.08
22	B	610	CLA	C3D-C4D-ND	2.08	113.36	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	402	CLA	C1D-CHD-C4C	-2.07	121.61	126.02
29	c	516	DGD	C3G-O3G-C1D	2.07	118.24	113.80
22	b	616	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
22	c	503	CLA	CHD-C4C-NC	2.07	127.44	124.23
22	B	611	CLA	CMB-C2B-C3B	2.07	131.42	126.55
22	C	504	CLA	CHB-C1B-NB	2.07	127.15	124.05
22	b	615	CLA	CHA-C4D-ND	2.07	136.82	132.55
22	B	612	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
22	b	608	CLA	CBA-CAA-C2A	2.07	119.95	113.79
31	B	625	STE	O1-C1-C2	-2.07	116.53	123.09
22	B	604	CLA	CHD-C1D-C2D	2.07	129.79	125.49
28	d	409	LHG	C29-C28-C27	-2.07	103.91	114.37
22	c	506	CLA	CAC-C3C-C4C	2.07	127.48	124.79
22	C	505	CLA	CMB-C2B-C3B	2.07	131.41	126.55
27	f	102	SQD	O5-C5-C4	2.07	113.42	109.70
30	k	102	BCR	C33-C5-C6	-2.06	122.23	124.48
23	D	401	PHO	C3D-C4D-ND	2.06	110.35	107.71
22	b	616	CLA	O2D-CGD-CBD	2.06	114.84	111.23
30	a	406	BCR	C21-C20-C19	-2.06	117.22	123.20
30	K	101	BCR	C15-C14-C13	-2.06	124.39	127.28
30	B	617	BCR	C38-C26-C25	-2.06	122.23	124.48
28	A	411	LHG	C20-C19-C18	-2.06	103.94	114.37
30	T	101	BCR	C30-C25-C26	-2.06	119.82	122.64
28	D	413	LHG	C18-C17-C16	-2.06	103.95	114.37
22	B	601	CLA	C16-C15-C13	-2.06	109.12	115.97
22	C	501	CLA	CAC-C3C-C4C	2.06	127.47	124.79
22	B	607	CLA	C3D-C4D-ND	2.06	113.33	109.99
30	k	101	BCR	C2-C1-C6	2.06	113.43	110.44
30	a	406	BCR	C33-C5-C6	-2.06	122.24	124.48
23	d	401	PHO	OBD-CAD-C3D	2.06	131.10	127.89
22	b	614	CLA	CBC-CAC-C3C	-2.06	106.84	112.42
22	C	505	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
22	b	605	CLA	CHC-C1C-NC	2.06	127.41	124.31
30	t	101	BCR	C34-C9-C10	-2.06	119.49	122.82
22	c	506	CLA	CMB-C2B-C1B	-2.05	122.29	125.42
22	C	504	CLA	C6-C5-C3	2.05	118.47	113.47
22	B	604	CLA	CHD-C4C-NC	2.05	127.42	124.23
22	C	507	CLA	C1C-C2C-C3C	-2.05	104.82	106.98
22	c	506	CLA	CHA-C1A-NA	-2.05	121.74	126.39
22	C	508	CLA	CMD-C2D-C1D	2.05	128.34	124.73
22	b	611	CLA	C1-O2A-CGA	-2.05	111.69	116.65
34	f	101	HEC	C1D-C2D-C3D	-2.05	104.82	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	516	DGD	O2D-C2D-C1D	-2.05	105.19	110.08
22	B	610	CLA	C9-C8-C10	-2.05	103.97	111.27
22	b	614	CLA	C1-C2-C3	-2.05	122.84	126.20
22	c	506	CLA	CHD-C4C-C3C	2.05	127.76	124.77
29	c	517	DGD	O5E-C6E-C5E	-2.05	104.36	111.33
34	f	101	HEC	C3B-C4B-NB	-2.05	107.92	110.17
22	C	503	CLA	CHB-C4A-NA	2.05	127.35	124.40
26	M	101	LMG	C37-C36-C35	-2.05	104.03	114.37
22	c	503	CLA	CHC-C1C-C2C	-2.05	121.14	126.95
28	b	623	LHG	O2-C2-C3	-2.04	102.63	109.70
22	c	501	CLA	C2C-C1C-NC	2.04	112.13	109.98
22	a	402	CLA	C4D-CHA-C1A	2.04	123.68	121.24
22	c	506	CLA	O2A-CGA-CBA	-2.04	105.60	111.83
26	c	518	LMG	C9-C8-C7	-2.04	107.02	111.78
29	H	103	DGD	C9A-C8A-C7A	-2.04	104.04	114.37
22	H	101	CLA	C4-C3-C5	2.04	118.77	115.23
22	b	614	CLA	C11-C10-C8	-2.04	109.18	115.97
28	D	413	LHG	O10-C23-C24	-2.04	115.80	123.78
22	C	512	CLA	C2A-C3A-C4A	2.04	105.17	101.87
22	b	607	CLA	C3B-C4B-NB	-2.04	108.71	110.53
22	A	402	CLA	C2D-C1D-ND	2.04	112.15	110.13
22	c	504	CLA	CMB-C2B-C3B	2.04	131.35	126.55
29	C	518	DGD	C8B-C7B-C6B	-2.04	104.06	114.37
29	H	103	DGD	C8B-C7B-C6B	-2.04	104.07	114.37
22	C	508	CLA	CHA-C4D-ND	2.04	136.75	132.55
29	h	101	DGD	CDB-CCB-CBB	-2.04	104.07	114.37
29	H	103	DGD	O2E-C2E-C3E	-2.04	105.57	110.38
22	b	602	CLA	CGD-CBD-CAD	-2.04	104.26	110.85
22	b	602	CLA	CHB-C1B-C2B	-2.04	121.52	127.43
30	b	618	BCR	C36-C18-C17	-2.04	119.52	122.82
30	B	618	BCR	C30-C25-C24	2.03	121.17	115.65
30	t	101	BCR	C1-C6-C7	2.03	121.17	115.65
22	b	614	CLA	CHA-C4D-ND	2.03	136.75	132.55
26	d	410	LMG	C40-C39-C38	-2.03	104.09	114.37
22	C	512	CLA	O2D-CGD-CBD	2.03	114.78	111.23
30	t	101	BCR	C11-C10-C9	-2.03	124.43	127.28
22	C	507	CLA	O1D-CGD-CBD	2.03	128.53	124.52
22	B	603	CLA	C1C-C2C-C3C	-2.03	104.84	106.98
28	L	102	LHG	C20-C19-C18	-2.03	104.10	114.37
22	b	611	CLA	C2D-C1D-ND	-2.03	108.12	110.13
27	B	621	SQD	C45-O47-C7	2.03	122.66	117.80
30	b	618	BCR	C27-C26-C25	2.03	125.45	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	409	PL9	C45-C44-C43	-2.03	118.42	123.63
22	B	610	CLA	CBC-CAC-C3C	-2.03	106.92	112.42
22	b	604	CLA	CBA-CAA-C2A	-2.03	107.76	113.79
22	C	509	CLA	C2A-C3A-C4A	2.03	105.14	101.87
22	b	616	CLA	CMB-C2B-C3B	2.03	131.32	126.55
29	c	517	DGD	C7B-C6B-C5B	-2.03	104.12	114.37
22	c	503	CLA	C3A-C2A-C1A	2.03	104.37	101.34
22	b	610	CLA	O2D-CGD-O1D	-2.03	119.91	123.85
30	C	515	BCR	C37-C22-C21	-2.03	119.53	122.82
25	D	407	PL9	C41-C39-C38	-2.02	116.63	121.17
28	A	411	LHG	C11-C10-C9	-2.02	104.14	114.37
30	I	101	BCR	C4-C5-C6	2.02	125.44	122.70
30	d	406	BCR	C10-C11-C12	-2.02	117.34	123.20
22	a	402	CLA	CHD-C1D-ND	-2.02	121.96	124.80
22	C	502	CLA	CHB-C1B-NB	2.02	127.08	124.05
22	c	510	CLA	CMB-C2B-C3B	2.02	131.31	126.55
22	C	504	CLA	C3B-C4B-NB	-2.02	108.73	110.53
25	d	407	PL9	C42-C43-C44	-2.02	123.00	127.62
22	c	504	CLA	C1C-C2C-C3C	-2.02	104.86	106.98
22	B	613	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
26	a	414	LMG	O6-C1-O1	-2.02	105.28	110.04
28	d	408	LHG	C27-C26-C25	-2.02	104.17	114.37
22	b	608	CLA	CHB-C1B-NB	2.02	127.08	124.05
30	C	514	BCR	C40-C30-C39	-2.01	102.86	108.63
27	f	102	SQD	O47-C7-C8	2.01	118.33	110.93
22	c	506	CLA	C3B-C4B-NB	-2.01	108.73	110.53
22	B	608	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
26	m	101	LMG	C38-C37-C36	-2.01	104.20	114.37
29	C	518	DGD	CDB-CCB-CBB	-2.01	104.20	114.37
22	b	614	CLA	CMB-C2B-C3B	2.01	131.28	126.55
22	b	609	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
22	B	601	CLA	CHC-C4B-NB	2.01	127.06	124.05
27	a	410	SQD	C45-O47-C7	2.01	122.60	117.80
22	A	403	CLA	CMB-C2B-C3B	2.01	131.28	126.55
27	f	102	SQD	C46-C45-C44	-2.01	107.10	111.78
22	c	511	CLA	C3A-C2A-C1A	2.01	104.35	101.34
22	D	404	CLA	C11-C12-C13	-2.01	109.29	115.97
22	B	611	CLA	CAA-CBA-CGA	-2.01	107.51	113.21
22	B	611	CLA	C4C-C3C-C2C	-2.01	103.97	106.89
27	A	410	SQD	O48-C46-C45	2.01	114.18	108.40
22	a	405	CLA	C2A-C1A-CHA	2.01	127.35	123.87
29	c	515	DGD	O3G-C1D-C2D	-2.00	105.23	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	406	BCR	C35-C13-C14	-2.00	119.57	122.82
30	B	617	BCR	C28-C27-C26	-2.00	110.48	114.06
22	c	511	CLA	O2D-CGD-CBD	2.00	114.73	111.23
22	C	510	CLA	CHD-C4C-NC	2.00	127.33	124.23
29	C	517	DGD	O5D-C6D-C5D	-2.00	104.91	109.42

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
34	F	101	HEC	NA
34	V	201	HEC	NA
34	f	101	HEC	NA
34	v	201	HEC	NA

All (1966) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	604	CLA	C6-C7-C8-C9
22	B	605	CLA	C2B-C3B-CAB-CBB
22	B	605	CLA	C4B-C3B-CAB-CBB
22	B	605	CLA	C11-C10-C8-C9
22	C	501	CLA	CBD-CGD-O2D-CED
22	C	502	CLA	CAD-CBD-CGD-O1D
22	C	502	CLA	CAD-CBD-CGD-O2D
22	C	502	CLA	C14-C13-C15-C16
22	C	507	CLA	CHA-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O2D
22	C	509	CLA	C2-C1-O2A-CGA
22	C	509	CLA	CHA-CBD-CGD-O1D
22	C	509	CLA	CHA-CBD-CGD-O2D
22	C	512	CLA	C1A-C2A-CAA-CBA
22	C	512	CLA	C2B-C3B-CAB-CBB
22	C	512	CLA	C4B-C3B-CAB-CBB
22	C	512	CLA	C11-C10-C8-C9
22	a	403	CLA	C2B-C3B-CAB-CBB
22	a	403	CLA	C4B-C3B-CAB-CBB
22	b	601	CLA	C1A-C2A-CAA-CBA
22	b	601	CLA	C4B-C3B-CAB-CBB
22	b	601	CLA	CBD-CGD-O2D-CED
22	b	609	CLA	C2B-C3B-CAB-CBB
22	b	609	CLA	C4B-C3B-CAB-CBB
22	b	614	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	CAD-CBD-CGD-O2D
22	b	614	CLA	CBD-CGD-O2D-CED
22	c	505	CLA	C2B-C3B-CAB-CBB
22	c	505	CLA	C4B-C3B-CAB-CBB
22	c	506	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	CBD-CGD-O2D-CED
22	c	512	CLA	C1A-C2A-CAA-CBA
22	c	512	CLA	C2B-C3B-CAB-CBB
22	c	512	CLA	C4B-C3B-CAB-CBB
22	c	512	CLA	C6-C7-C8-C9
22	c	513	CLA	C1A-C2A-CAA-CBA
22	c	513	CLA	C3A-C2A-CAA-CBA
25	A	408	PL9	C17-C18-C19-C20
25	A	408	PL9	C24-C26-C27-C28
25	A	408	PL9	C32-C33-C34-C36
25	A	408	PL9	C34-C36-C37-C38
25	A	408	PL9	C37-C38-C39-C40
25	D	407	PL9	C42-C43-C44-C45
25	D	407	PL9	C47-C48-C49-C51
25	a	409	PL9	C12-C13-C14-C15
25	a	409	PL9	C12-C13-C14-C16
25	a	409	PL9	C17-C18-C19-C21
25	a	409	PL9	C27-C28-C29-C30
25	a	409	PL9	C32-C33-C34-C35
25	a	409	PL9	C37-C38-C39-C40
25	a	409	PL9	C42-C43-C44-C45
25	a	409	PL9	C42-C43-C44-C46
25	d	407	PL9	C27-C28-C29-C31
25	d	407	PL9	C32-C33-C34-C36
25	d	407	PL9	C37-C38-C39-C41
25	d	407	PL9	C42-C43-C44-C46
25	d	407	PL9	C47-C48-C49-C50
26	A	409	LMG	O9-C10-O7-C8
26	b	622	LMG	C11-C10-O7-C8
26	c	521	LMG	O6-C1-O1-C7
27	A	412	SQD	C46-C45-O47-C7
27	B	621	SQD	C2-C1-O6-C44
27	B	621	SQD	O5-C1-O6-C44
27	B	621	SQD	O6-C44-C45-O47
27	B	621	SQD	O49-C7-O47-C45
27	B	621	SQD	C8-C7-O47-C45
27	L	101	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
27	f	102	SQD	C2-C1-O6-C44
27	f	102	SQD	O5-C1-O6-C44
27	t	102	SQD	O49-C7-O47-C45
27	t	102	SQD	C8-C7-O47-C45
28	A	411	LHG	O1-C1-C2-C3
28	A	411	LHG	C3-O3-P-O5
28	A	411	LHG	C3-O3-P-O6
28	A	411	LHG	C4-O6-P-O3
28	D	410	LHG	O1-C1-C2-C3
28	D	410	LHG	C3-O3-P-O5
28	D	410	LHG	C3-O3-P-O6
28	D	410	LHG	C4-O6-P-O4
28	D	411	LHG	C3-O3-P-O5
28	D	411	LHG	C3-O3-P-O6
28	D	413	LHG	O1-C1-C2-O2
28	D	413	LHG	O1-C1-C2-C3
28	D	413	LHG	C1-C2-C3-O3
28	L	102	LHG	C3-O3-P-O4
28	L	102	LHG	C3-O3-P-O6
28	L	102	LHG	C4-O6-P-O4
28	a	411	LHG	O1-C1-C2-O2
28	a	411	LHG	O1-C1-C2-C3
28	a	411	LHG	C3-O3-P-O4
28	a	411	LHG	C3-O3-P-O6
28	a	411	LHG	O6-C4-C5-O7
28	a	411	LHG	O10-C23-O8-C6
28	a	411	LHG	C24-C23-O8-C6
28	b	623	LHG	O1-C1-C2-C3
28	b	623	LHG	C3-O3-P-O4
28	b	623	LHG	C4-O6-P-O3
28	b	623	LHG	C4-O6-P-O4
28	d	408	LHG	O1-C1-C2-C3
28	d	408	LHG	C3-O3-P-O4
28	d	408	LHG	C3-O3-P-O6
28	d	408	LHG	C4-O6-P-O3
28	d	408	LHG	C4-O6-P-O4
28	l	101	LHG	C4-O6-P-O4
29	A	413	DGD	C2B-C1B-O2G-C2G
29	A	413	DGD	O1B-C1B-O2G-C2G
29	A	413	DGD	O2G-C2G-C3G-O3G
30	B	616	BCR	C35-C13-C14-C15
30	B	616	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
30	B	616	BCR	C20-C21-C22-C37
30	B	617	BCR	C11-C10-C9-C34
30	B	617	BCR	C10-C11-C12-C13
30	B	617	BCR	C37-C22-C23-C24
30	B	618	BCR	C11-C10-C9-C8
30	B	618	BCR	C35-C13-C14-C15
30	C	514	BCR	C1-C6-C7-C8
30	C	514	BCR	C5-C6-C7-C8
30	C	514	BCR	C7-C8-C9-C10
30	C	515	BCR	C11-C12-C13-C14
30	D	406	BCR	C7-C8-C9-C10
30	D	406	BCR	C11-C10-C9-C34
30	D	406	BCR	C22-C23-C24-C25
30	H	102	BCR	C11-C12-C13-C14
30	H	102	BCR	C36-C18-C19-C20
30	I	101	BCR	C11-C10-C9-C34
30	I	101	BCR	C11-C12-C13-C35
30	I	101	BCR	C14-C15-C16-C17
30	I	101	BCR	C16-C17-C18-C19
30	I	101	BCR	C20-C21-C22-C37
30	K	101	BCR	C6-C7-C8-C9
30	K	101	BCR	C7-C8-C9-C34
30	K	101	BCR	C11-C10-C9-C8
30	K	101	BCR	C14-C15-C16-C17
30	K	101	BCR	C16-C17-C18-C36
30	K	102	BCR	C1-C6-C7-C8
30	K	102	BCR	C5-C6-C7-C8
30	K	102	BCR	C11-C10-C9-C34
30	K	102	BCR	C11-C12-C13-C14
30	K	102	BCR	C16-C17-C18-C36
30	K	102	BCR	C21-C22-C23-C24
30	K	102	BCR	C37-C22-C23-C24
30	T	101	BCR	C7-C8-C9-C10
30	T	101	BCR	C9-C10-C11-C12
30	T	101	BCR	C11-C12-C13-C14
30	a	406	BCR	C37-C22-C23-C24
30	b	617	BCR	C11-C10-C9-C8
30	b	617	BCR	C12-C13-C14-C15
30	b	617	BCR	C35-C13-C14-C15
30	b	617	BCR	C20-C21-C22-C37
30	b	617	BCR	C21-C22-C23-C24
30	c	514	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
30	c	514	BCR	C12-C13-C14-C15
30	c	514	BCR	C16-C17-C18-C36
30	d	406	BCR	C35-C13-C14-C15
30	d	406	BCR	C37-C22-C23-C24
30	d	406	BCR	C22-C23-C24-C25
30	k	101	BCR	C6-C7-C8-C9
30	k	101	BCR	C7-C8-C9-C10
30	k	101	BCR	C35-C13-C14-C15
30	k	101	BCR	C18-C19-C20-C21
30	k	101	BCR	C20-C21-C22-C37
30	k	102	BCR	C7-C8-C9-C10
30	k	102	BCR	C7-C8-C9-C34
30	k	102	BCR	C17-C18-C19-C20
30	k	102	BCR	C21-C22-C23-C24
30	t	101	BCR	C11-C10-C9-C34
30	t	101	BCR	C35-C13-C14-C15
30	t	101	BCR	C16-C17-C18-C19
30	t	101	BCR	C16-C17-C18-C36
34	V	201	HEC	C2C-C3C-CAC-CBC
34	F	101	HEC	C4B-C3B-CAB-CBB
22	b	614	CLA	O1D-CGD-O2D-CED
34	F	101	HEC	C2B-C3B-CAB-CBB
22	C	509	CLA	O1D-CGD-O2D-CED
22	b	613	CLA	O1D-CGD-O2D-CED
22	C	509	CLA	CBD-CGD-O2D-CED
22	H	101	CLA	CBD-CGD-O2D-CED
22	b	613	CLA	CBD-CGD-O2D-CED
22	c	510	CLA	CBD-CGD-O2D-CED
22	c	513	CLA	CBD-CGD-O2D-CED
26	c	520	LMG	O10-C28-O8-C9
26	c	521	LMG	O10-C28-O8-C9
26	c	518	LMG	C11-C10-O7-C8
34	F	101	HEC	C2C-C3C-CAC-CBC
34	V	201	HEC	C4C-C3C-CAC-CBC
25	D	407	PL9	C47-C48-C49-C50
25	a	409	PL9	C47-C48-C49-C50
25	a	409	PL9	C47-C48-C49-C51
25	d	407	PL9	C47-C48-C49-C51
22	B	603	CLA	O1A-CGA-O2A-C1
22	H	101	CLA	O1A-CGA-O2A-C1
27	L	101	SQD	O10-C23-O48-C46
34	F	101	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
22	c	506	CLA	O1D-CGD-O2D-CED
22	c	508	CLA	O1D-CGD-O2D-CED
22	b	601	CLA	O1D-CGD-O2D-CED
26	c	518	LMG	O9-C10-O7-C8
26	M	101	LMG	O10-C28-O8-C9
26	D	412	LMG	O9-C10-O7-C8
26	Y	101	LMG	O9-C10-O7-C8
26	b	622	LMG	O9-C10-O7-C8
27	f	102	SQD	O49-C7-O47-C45
22	B	603	CLA	C3-C5-C6-C7
22	B	604	CLA	C3-C5-C6-C7
22	b	601	CLA	C3-C5-C6-C7
22	c	510	CLA	C3-C5-C6-C7
22	H	101	CLA	O1D-CGD-O2D-CED
26	c	521	LMG	C29-C28-O8-C9
27	L	101	SQD	C24-C23-O48-C46
27	f	102	SQD	C24-C23-O48-C46
22	B	615	CLA	CBD-CGD-O2D-CED
22	b	607	CLA	CBD-CGD-O2D-CED
22	c	512	CLA	CBD-CGD-O2D-CED
26	A	409	LMG	C11-C10-O7-C8
26	D	412	LMG	C11-C10-O7-C8
26	Y	101	LMG	C11-C10-O7-C8
26	c	520	LMG	C11-C10-O7-C8
27	L	101	SQD	C8-C7-O47-C45
22	C	501	CLA	O1D-CGD-O2D-CED
34	f	101	HEC	C2B-C3B-CAB-CBB
22	B	602	CLA	C4-C3-C5-C6
22	B	603	CLA	C4-C3-C5-C6
22	B	613	CLA	C4-C3-C5-C6
22	b	604	CLA	C4-C3-C5-C6
22	b	605	CLA	C4-C3-C5-C6
22	b	614	CLA	C4-C3-C5-C6
22	c	504	CLA	C4-C3-C5-C6
25	A	408	PL9	C40-C39-C41-C42
22	B	602	CLA	C2-C3-C5-C6
22	B	603	CLA	C2-C3-C5-C6
22	B	613	CLA	C2-C3-C5-C6
22	b	604	CLA	C2-C3-C5-C6
22	b	605	CLA	C2-C3-C5-C6
22	b	614	CLA	C2-C3-C5-C6
22	c	504	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	A	408	PL9	C23-C24-C26-C27
25	A	408	PL9	C43-C44-C46-C47
25	d	407	PL9	C38-C39-C41-C42
22	c	510	CLA	O1D-CGD-O2D-CED
22	c	513	CLA	O1D-CGD-O2D-CED
34	f	101	HEC	C4C-C3C-CAC-CBC
34	v	201	HEC	C4C-C3C-CAC-CBC
22	d	405	CLA	C3-C5-C6-C7
22	B	603	CLA	CBA-CGA-O2A-C1
22	H	101	CLA	CBA-CGA-O2A-C1
26	a	414	LMG	C29-C28-O8-C9
26	c	520	LMG	C29-C28-O8-C9
25	a	409	PL9	C17-C18-C19-C20
25	A	408	PL9	C22-C23-C24-C26
25	A	408	PL9	C37-C38-C39-C41
25	D	407	PL9	C32-C33-C34-C36
25	a	409	PL9	C37-C38-C39-C41
26	c	520	LMG	O9-C10-O7-C8
29	h	101	DGD	O6E-C5E-C6E-O5E
22	b	609	CLA	C3-C5-C6-C7
22	b	614	CLA	C3-C5-C6-C7
22	B	613	CLA	CBD-CGD-O2D-CED
22	b	603	CLA	CBD-CGD-O2D-CED
28	D	413	LHG	O2-C2-C3-O3
26	M	101	LMG	C29-C28-O8-C9
26	A	409	LMG	C4-C5-C6-O5
22	B	611	CLA	CBD-CGD-O2D-CED
34	f	101	HEC	C4B-C3B-CAB-CBB
22	b	605	CLA	CBD-CGD-O2D-CED
26	A	409	LMG	O6-C5-C6-O5
29	h	101	DGD	C4E-C5E-C6E-O5E
22	C	504	CLA	C4-C3-C5-C6
22	C	504	CLA	C2-C3-C5-C6
26	a	414	LMG	O10-C28-O8-C9
27	f	102	SQD	O10-C23-O48-C46
29	c	517	DGD	O1A-C1A-O1G-C1G
25	A	408	PL9	C29-C31-C32-C33
25	D	407	PL9	C34-C36-C37-C38
25	D	407	PL9	C44-C46-C47-C48
25	a	409	PL9	C9-C11-C12-C13
25	a	409	PL9	C14-C16-C17-C18
25	a	409	PL9	C19-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
25	a	409	PL9	C24-C26-C27-C28
25	d	407	PL9	C44-C46-C47-C48
27	D	409	SQD	O10-C23-O48-C46
22	C	502	CLA	CBD-CGD-O2D-CED
26	Y	101	LMG	O6-C5-C6-O5
25	A	408	PL9	C7-C8-C9-C10
25	a	409	PL9	C22-C23-C24-C26
34	f	101	HEC	C2C-C3C-CAC-CBC
22	c	501	CLA	CBD-CGD-O2D-CED
31	B	624	STE	C11-C12-C13-C14
28	a	411	LHG	C1-C2-C3-O3
27	B	621	SQD	C24-C23-O48-C46
27	D	409	SQD	C24-C23-O48-C46
22	b	609	CLA	CBD-CGD-O2D-CED
31	b	621	STE	C14-C15-C16-C17
22	B	615	CLA	O1D-CGD-O2D-CED
31	a	413	STE	C5-C6-C7-C8
25	a	409	PL9	C28-C29-C31-C32
22	B	606	CLA	C14-C13-C15-C16
22	B	613	CLA	C11-C12-C13-C14
22	B	613	CLA	C14-C13-C15-C16
22	C	503	CLA	C11-C10-C8-C9
22	C	509	CLA	C11-C10-C8-C9
22	D	405	CLA	C11-C12-C13-C14
22	H	101	CLA	C6-C7-C8-C9
22	b	601	CLA	C11-C10-C8-C9
22	b	605	CLA	C11-C10-C8-C9
22	b	607	CLA	C11-C10-C8-C9
22	b	613	CLA	C11-C12-C13-C14
22	b	614	CLA	C6-C7-C8-C9
22	b	616	CLA	C11-C10-C8-C9
22	c	503	CLA	C11-C12-C13-C14
22	c	509	CLA	C6-C7-C8-C9
22	d	405	CLA	C11-C12-C13-C14
23	A	404	PHO	C14-C13-C15-C16
26	B	620	LMG	C28-C29-C30-C31
28	D	411	LHG	O2-C2-C3-O3
28	a	411	LHG	O2-C2-C3-O3
30	B	618	BCR	C7-C8-C9-C34
30	C	514	BCR	C7-C8-C9-C34
30	C	515	BCR	C7-C8-C9-C34
30	C	515	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
30	D	406	BCR	C37-C22-C23-C24
30	H	102	BCR	C37-C22-C23-C24
30	K	101	BCR	C36-C18-C19-C20
30	K	102	BCR	C11-C12-C13-C35
30	T	101	BCR	C7-C8-C9-C34
30	T	101	BCR	C11-C12-C13-C35
30	b	617	BCR	C7-C8-C9-C34
30	b	617	BCR	C11-C12-C13-C35
30	b	619	BCR	C11-C12-C13-C35
30	k	101	BCR	C7-C8-C9-C34
30	k	102	BCR	C11-C12-C13-C35
30	k	102	BCR	C37-C22-C23-C24
30	k	103	BCR	C37-C22-C23-C24
22	C	512	CLA	C3-C5-C6-C7
22	c	507	CLA	C5-C6-C7-C8
22	c	510	CLA	C5-C6-C7-C8
22	c	512	CLA	C13-C15-C16-C17
26	d	410	LMG	C10-C11-C12-C13
22	b	607	CLA	O1D-CGD-O2D-CED
22	C	510	CLA	CBD-CGD-O2D-CED
22	B	610	CLA	C13-C15-C16-C17
22	C	506	CLA	C15-C16-C17-C18
26	c	518	LMG	C28-C29-C30-C31
29	C	516	DGD	O6E-C5E-C6E-O5E
22	B	605	CLA	C12-C13-C15-C16
22	b	608	CLA	C11-C12-C13-C15
22	b	613	CLA	C11-C10-C8-C7
22	d	405	CLA	C6-C7-C8-C10
25	a	409	PL9	C30-C29-C31-C32
22	c	510	CLA	C10-C11-C12-C13
31	b	624	STE	C1-C2-C3-C4
25	A	408	PL9	C47-C48-C49-C50
25	A	408	PL9	C44-C46-C47-C48
28	d	409	LHG	C24-C25-C26-C27
22	c	505	CLA	C15-C16-C17-C18
26	D	408	LMG	C10-C11-C12-C13
26	Y	101	LMG	C28-C29-C30-C31
26	a	414	LMG	C10-C11-C12-C13
28	l	101	LHG	C23-C24-C25-C26
31	B	623	STE	C1-C2-C3-C4
31	x	102	STE	C1-C2-C3-C4
26	m	101	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
22	B	606	CLA	CBD-CGD-O2D-CED
22	B	602	CLA	C8-C10-C11-C12
22	C	502	CLA	C15-C16-C17-C18
22	C	510	CLA	C13-C15-C16-C17
22	c	511	CLA	C15-C16-C17-C18
22	B	605	CLA	C2A-CAA-CBA-CGA
22	b	601	CLA	C2A-CAA-CBA-CGA
22	c	513	CLA	C2A-CAA-CBA-CGA
30	T	101	BCR	C18-C19-C20-C21
22	B	604	CLA	C8-C10-C11-C12
22	B	606	CLA	C8-C10-C11-C12
22	B	612	CLA	C8-C10-C11-C12
22	b	615	CLA	C8-C10-C11-C12
26	M	101	LMG	C28-C29-C30-C31
28	d	409	LHG	C23-C24-C25-C26
29	C	517	DGD	C1B-C2B-C3B-C4B
29	c	515	DGD	C1B-C2B-C3B-C4B
31	L	103	STE	C1-C2-C3-C4
22	b	602	CLA	CBD-CGD-O2D-CED
22	b	610	CLA	CBD-CGD-O2D-CED
26	Y	101	LMG	O6-C1-O1-C7
26	b	622	LMG	O6-C1-O1-C7
29	A	413	DGD	O6E-C1E-O5D-C6D
30	b	617	BCR	C6-C7-C8-C9
22	B	613	CLA	O1D-CGD-O2D-CED
22	B	603	CLA	C5-C6-C7-C8
22	B	607	CLA	C15-C16-C17-C18
22	B	608	CLA	C15-C16-C17-C18
22	B	613	CLA	C8-C10-C11-C12
22	C	503	CLA	C5-C6-C7-C8
22	C	505	CLA	C10-C11-C12-C13
22	C	508	CLA	C15-C16-C17-C18
22	a	405	CLA	C5-C6-C7-C8
22	b	605	CLA	C5-C6-C7-C8
31	c	519	STE	C2-C3-C4-C5
22	C	506	CLA	CBD-CGD-O2D-CED
26	M	101	LMG	C10-C11-C12-C13
31	B	625	STE	C1-C2-C3-C4
22	B	604	CLA	C15-C16-C17-C18
22	C	506	CLA	C8-C10-C11-C12
29	H	103	DGD	C4E-C5E-C6E-O5E
25	D	407	PL9	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
22	C	505	CLA	C5-C6-C7-C8
22	C	509	CLA	C10-C11-C12-C13
22	C	512	CLA	C8-C10-C11-C12
22	D	405	CLA	C10-C11-C12-C13
22	b	608	CLA	C13-C15-C16-C17
22	c	509	CLA	C10-C11-C12-C13
25	a	409	PL9	C38-C39-C41-C42
29	A	413	DGD	O6D-C5D-C6D-O5D
27	A	410	SQD	C7-C8-C9-C10
22	c	512	CLA	O1D-CGD-O2D-CED
22	b	615	CLA	C5-C6-C7-C8
22	c	512	CLA	CBA-CGA-O2A-C1
27	a	410	SQD	C24-C23-O48-C46
34	v	201	HEC	C2C-C3C-CAC-CBC
34	V	201	HEC	C2B-C3B-CAB-CBB
22	d	405	CLA	CBD-CGD-O2D-CED
27	B	621	SQD	C23-C24-C25-C26
22	b	606	CLA	C2A-CAA-CBA-CGA
22	c	512	CLA	C2A-CAA-CBA-CGA
29	c	517	DGD	C2A-C1A-O1G-C1G
28	d	409	LHG	C30-C31-C32-C33
22	B	606	CLA	C5-C6-C7-C8
22	C	513	CLA	C13-C15-C16-C17
22	C	513	CLA	C15-C16-C17-C18
22	b	611	CLA	C15-C16-C17-C18
26	Y	101	LMG	C4-C5-C6-O5
31	b	626	STE	C4-C5-C6-C7
22	B	605	CLA	C8-C10-C11-C12
22	D	403	CLA	C15-C16-C17-C18
22	b	606	CLA	C10-C11-C12-C13
22	b	614	CLA	C13-C15-C16-C17
22	C	509	CLA	C13-C15-C16-C17
22	C	510	CLA	C15-C16-C17-C18
22	b	603	CLA	C10-C11-C12-C13
22	b	611	CLA	C10-C11-C12-C13
22	b	614	CLA	C8-C10-C11-C12
22	c	511	CLA	C13-C15-C16-C17
26	d	410	LMG	C28-C29-C30-C31
22	b	616	CLA	C10-C11-C12-C13
22	b	602	CLA	C3-C5-C6-C7
22	B	603	CLA	CBD-CGD-O2D-CED
26	Y	101	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
26	b	622	LMG	C2-C1-O1-C7
26	m	101	LMG	C2-C1-O1-C7
29	A	413	DGD	C2E-C1E-O5D-C6D
29	C	517	DGD	C2E-C1E-O5D-C6D
29	c	516	DGD	C2E-C1E-O5D-C6D
22	c	507	CLA	C8-C10-C11-C12
22	c	503	CLA	C16-C17-C18-C20
30	B	618	BCR	C11-C10-C9-C34
30	C	514	BCR	C16-C17-C18-C36
30	C	515	BCR	C11-C10-C9-C34
30	C	515	BCR	C20-C21-C22-C37
30	D	406	BCR	C35-C13-C14-C15
30	D	406	BCR	C20-C21-C22-C37
30	I	101	BCR	C16-C17-C18-C36
30	K	101	BCR	C20-C21-C22-C37
30	T	101	BCR	C16-C17-C18-C36
30	b	619	BCR	C35-C13-C14-C15
30	d	406	BCR	C20-C21-C22-C37
30	t	101	BCR	C20-C21-C22-C37
30	x	101	BCR	C11-C10-C9-C34
29	C	518	DGD	C8A-C9A-CAA-CBA
30	B	618	BCR	C37-C22-C23-C24
30	H	102	BCR	C7-C8-C9-C34
30	T	101	BCR	C37-C22-C23-C24
26	D	412	LMG	O10-C28-O8-C9
22	D	404	CLA	C13-C15-C16-C17
28	d	409	LHG	O1-C1-C2-C3
26	D	412	LMG	C28-C29-C30-C31
27	L	101	SQD	C46-C45-O47-C7
31	B	625	STE	C5-C6-C7-C8
22	B	605	CLA	C16-C17-C18-C20
22	B	609	CLA	C16-C17-C18-C20
22	b	601	CLA	C16-C17-C18-C20
22	b	605	CLA	C16-C17-C18-C19
22	b	613	CLA	C16-C17-C18-C19
23	D	401	PHO	C16-C17-C18-C19
22	B	611	CLA	O1D-CGD-O2D-CED
22	b	605	CLA	O1D-CGD-O2D-CED
30	B	616	BCR	C12-C13-C14-C15
30	B	616	BCR	C16-C17-C18-C19
30	B	616	BCR	C20-C21-C22-C23
30	B	617	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
30	C	515	BCR	C11-C10-C9-C8
30	K	101	BCR	C16-C17-C18-C19
30	K	102	BCR	C11-C10-C9-C8
30	K	102	BCR	C16-C17-C18-C19
30	T	101	BCR	C12-C13-C14-C15
30	a	406	BCR	C20-C21-C22-C23
30	k	101	BCR	C20-C21-C22-C23
30	k	103	BCR	C16-C17-C18-C19
30	k	103	BCR	C20-C21-C22-C23
30	t	101	BCR	C11-C10-C9-C8
30	t	101	BCR	C12-C13-C14-C15
30	x	101	BCR	C11-C10-C9-C8
30	x	101	BCR	C16-C17-C18-C19
26	m	101	LMG	O6-C1-O1-C7
29	c	516	DGD	O6E-C1E-O5D-C6D
26	a	414	LMG	C11-C10-O7-C8
22	b	613	CLA	C13-C15-C16-C17
29	A	413	DGD	C4D-C5D-C6D-O5D
22	b	614	CLA	CBA-CGA-O2A-C1
22	c	506	CLA	C2-C1-O2A-CGA
22	b	614	CLA	C16-C17-C18-C20
22	c	510	CLA	C16-C17-C18-C19
22	c	512	CLA	O1A-CGA-O2A-C1
26	Y	101	LMG	O10-C28-O8-C9
22	b	611	CLA	C8-C10-C11-C12
26	b	622	LMG	C11-C12-C13-C14
26	c	520	LMG	C15-C16-C17-C18
29	A	413	DGD	C2B-C3B-C4B-C5B
29	C	518	DGD	CBA-CCA-CDA-CEA
29	h	101	DGD	C5B-C6B-C7B-C8B
31	R	101	STE	C2-C3-C4-C5
26	D	408	LMG	C17-C18-C19-C20
26	Y	101	LMG	C31-C32-C33-C34
26	c	521	LMG	C11-C12-C13-C14
27	B	621	SQD	C11-C10-C9-C8
27	a	410	SQD	C9-C10-C11-C12
28	A	411	LHG	C26-C27-C28-C29
28	D	410	LHG	C29-C30-C31-C32
28	D	413	LHG	C9-C10-C11-C12
29	A	413	DGD	CEA-CFA-CGA-CHA
29	c	515	DGD	C3B-C4B-C5B-C6B
31	I	102	STE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	b	628	STE	C11-C12-C13-C14
22	C	510	CLA	C10-C11-C12-C13
22	a	403	CLA	C13-C15-C16-C17
22	c	506	CLA	C10-C11-C12-C13
26	c	521	LMG	C34-C35-C36-C37
28	D	410	LHG	C28-C29-C30-C31
29	C	518	DGD	C4B-C5B-C6B-C7B
26	c	520	LMG	C34-C35-C36-C37
27	a	410	SQD	C10-C11-C12-C13
28	D	411	LHG	C12-C13-C14-C15
28	L	102	LHG	C30-C31-C32-C33
28	b	623	LHG	C32-C33-C34-C35
28	d	408	LHG	C29-C30-C31-C32
29	A	413	DGD	CBA-CCA-CDA-CEA
31	J	101	STE	C6-C7-C8-C9
31	L	103	STE	C3-C4-C5-C6
31	b	620	STE	C4-C5-C6-C7
31	b	621	STE	C11-C12-C13-C14
28	a	411	LHG	O9-C7-O7-C5
28	D	410	LHG	O1-C1-C2-O2
28	d	408	LHG	O1-C1-C2-O2
27	A	410	SQD	C25-C26-C27-C28
27	A	412	SQD	C24-C25-C26-C27
27	D	409	SQD	C25-C26-C27-C28
28	L	102	LHG	C31-C32-C33-C34
28	d	408	LHG	C11-C12-C13-C14
29	c	516	DGD	CCB-CDB-CEB-CFB
22	b	603	CLA	O1D-CGD-O2D-CED
22	d	405	CLA	O1D-CGD-O2D-CED
22	B	614	CLA	C4B-C3B-CAB-CBB
22	b	603	CLA	C4B-C3B-CAB-CBB
27	A	412	SQD	C7-C8-C9-C10
27	L	101	SQD	C7-C8-C9-C10
27	B	621	SQD	C11-C12-C13-C14
27	f	102	SQD	C30-C31-C32-C33
31	Z	101	STE	C13-C14-C15-C16
31	a	413	STE	C7-C8-C9-C10
29	H	103	DGD	O6E-C5E-C6E-O5E
22	B	612	CLA	C16-C17-C18-C20
22	D	404	CLA	C16-C17-C18-C20
22	b	604	CLA	C16-C17-C18-C19
22	b	605	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	C16-C17-C18-C19
27	t	102	SQD	C15-C16-C17-C18
29	A	413	DGD	CCB-CDB-CEB-CFB
31	B	622	STE	C6-C7-C8-C9
22	a	405	CLA	C10-C11-C12-C13
22	b	607	CLA	C10-C11-C12-C13
22	b	608	CLA	C8-C10-C11-C12
27	f	102	SQD	C8-C7-O47-C45
28	D	410	LHG	C15-C16-C17-C18
22	b	615	CLA	C11-C12-C13-C15
29	C	517	DGD	C6A-C7A-C8A-C9A
31	a	413	STE	C11-C10-C9-C8
31	b	628	STE	C9-C10-C11-C12
26	a	414	LMG	C12-C13-C14-C15
26	c	521	LMG	C30-C31-C32-C33
27	A	410	SQD	C14-C15-C16-C17
28	A	411	LHG	C32-C33-C34-C35
29	c	516	DGD	C8A-C9A-CAA-CBA
29	c	517	DGD	CCB-CDB-CEB-CFB
31	b	629	STE	C12-C13-C14-C15
31	x	102	STE	C9-C10-C11-C12
22	C	512	CLA	C3A-C2A-CAA-CBA
22	c	512	CLA	C3A-C2A-CAA-CBA
22	B	606	CLA	O1D-CGD-O2D-CED
22	C	502	CLA	O1D-CGD-O2D-CED
26	m	101	LMG	C17-C18-C19-C20
28	D	410	LHG	C17-C18-C19-C20
31	B	623	STE	C10-C11-C12-C13
31	B	624	STE	C9-C10-C11-C12
31	M	104	STE	C4-C5-C6-C7
31	b	629	STE	C4-C5-C6-C7
28	L	102	LHG	C24-C25-C26-C27
31	d	411	STE	C11-C12-C13-C14
22	A	403	CLA	C15-C16-C17-C18
22	b	607	CLA	C8-C10-C11-C12
22	b	609	CLA	O1D-CGD-O2D-CED
30	K	101	BCR	C15-C16-C17-C18
30	t	101	BCR	C15-C16-C17-C18
22	H	101	CLA	C16-C17-C18-C19
22	H	101	CLA	C16-C17-C18-C20
22	b	604	CLA	C16-C17-C18-C20
23	D	401	PHO	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
26	a	414	LMG	C33-C34-C35-C36
26	c	521	LMG	C32-C33-C34-C35
27	D	409	SQD	C30-C31-C32-C33
27	t	102	SQD	C11-C10-C9-C8
28	D	413	LHG	C15-C16-C17-C18
29	h	101	DGD	C2B-C3B-C4B-C5B
31	b	628	STE	C13-C14-C15-C16
26	c	518	LMG	C33-C34-C35-C36
27	L	101	SQD	C13-C14-C15-C16
28	D	410	LHG	C11-C12-C13-C14
29	c	517	DGD	C4B-C5B-C6B-C7B
26	c	520	LMG	O6-C5-C6-O5
27	A	410	SQD	C24-C23-O48-C46
26	a	414	LMG	O1-C7-C8-C9
26	c	521	LMG	C17-C18-C19-C20
26	d	410	LMG	C14-C15-C16-C17
27	A	410	SQD	C30-C31-C32-C33
28	A	411	LHG	C28-C29-C30-C31
28	l	101	LHG	C9-C10-C11-C12
31	B	622	STE	C2-C3-C4-C5
31	C	519	STE	C5-C6-C7-C8
31	b	620	STE	C6-C7-C8-C9
31	b	621	STE	C3-C4-C5-C6
28	d	408	LHG	C7-C8-C9-C10
22	c	507	CLA	C13-C15-C16-C17
26	D	408	LMG	C30-C31-C32-C33
26	c	518	LMG	C31-C32-C33-C34
27	B	621	SQD	C17-C18-C19-C20
27	L	101	SQD	C12-C13-C14-C15
27	L	101	SQD	C24-C25-C26-C27
27	a	410	SQD	C12-C13-C14-C15
27	a	410	SQD	C26-C27-C28-C29
29	c	515	DGD	C4A-C5A-C6A-C7A
29	c	515	DGD	C4B-C5B-C6B-C7B
27	A	412	SQD	C12-C13-C14-C15
27	t	102	SQD	C30-C31-C32-C33
28	D	411	LHG	C25-C26-C27-C28
28	D	411	LHG	C32-C33-C34-C35
28	d	408	LHG	C33-C34-C35-C36
31	B	623	STE	C4-C5-C6-C7
31	c	519	STE	C9-C10-C11-C12
31	k	104	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	x	102	STE	C4-C5-C6-C7
29	C	516	DGD	C6B-C7B-C8B-C9B
31	b	624	STE	C3-C4-C5-C6
26	M	101	LMG	C37-C38-C39-C40
28	D	411	LHG	C24-C25-C26-C27
29	A	413	DGD	CBB-CCB-CDB-CEB
29	C	517	DGD	C9B-CAB-CBB-CCB
22	c	510	CLA	C16-C17-C18-C20
22	b	601	CLA	C2B-C3B-CAB-CBB
30	B	617	BCR	C23-C24-C25-C26
30	B	617	BCR	C23-C24-C25-C30
30	D	406	BCR	C23-C24-C25-C26
30	D	406	BCR	C23-C24-C25-C30
30	H	102	BCR	C23-C24-C25-C26
30	H	102	BCR	C23-C24-C25-C30
30	T	101	BCR	C1-C6-C7-C8
29	c	517	DGD	C6B-C7B-C8B-C9B
31	b	628	STE	C10-C11-C12-C13
26	c	521	LMG	C11-C10-O7-C8
22	a	403	CLA	C8-C10-C11-C12
22	c	508	CLA	C10-C11-C12-C13
26	D	412	LMG	C14-C15-C16-C17
26	a	414	LMG	C13-C14-C15-C16
26	c	520	LMG	C30-C31-C32-C33
28	d	408	LHG	C14-C15-C16-C17
31	b	625	STE	C9-C10-C11-C12
31	x	102	STE	C3-C4-C5-C6
26	A	409	LMG	C36-C37-C38-C39
26	c	518	LMG	C38-C39-C40-C41
26	c	518	LMG	C39-C40-C41-C42
27	A	412	SQD	C10-C11-C12-C13
28	a	411	LHG	C27-C28-C29-C30
28	D	411	LHG	C11-C12-C13-C14
28	D	411	LHG	C16-C17-C18-C19
28	l	101	LHG	C28-C29-C30-C31
29	C	518	DGD	C6B-C7B-C8B-C9B
31	M	104	STE	C2-C3-C4-C5
25	d	407	PL9	C4-C3-C7-C8
26	a	414	LMG	C22-C23-C24-C25
26	a	414	LMG	C39-C40-C41-C42
27	D	409	SQD	C29-C30-C31-C32
28	b	623	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	A	413	DGD	C2A-C3A-C4A-C5A
27	B	621	SQD	C28-C29-C30-C31
29	C	517	DGD	C3B-C4B-C5B-C6B
30	C	515	BCR	C18-C19-C20-C21
30	k	102	BCR	C10-C11-C12-C13
30	k	103	BCR	C18-C19-C20-C21
30	t	101	BCR	C10-C11-C12-C13
22	D	404	CLA	C16-C17-C18-C19
26	M	101	LMG	C12-C13-C14-C15
26	c	521	LMG	C37-C38-C39-C40
27	t	102	SQD	C11-C12-C13-C14
28	l	101	LHG	C15-C16-C17-C18
29	A	413	DGD	C5B-C6B-C7B-C8B
29	c	516	DGD	C2A-C3A-C4A-C5A
31	H	104	STE	C4-C5-C6-C7
31	b	624	STE	C11-C10-C9-C8
22	A	403	CLA	C14-C13-C15-C16
27	f	102	SQD	C27-C28-C29-C30
27	A	410	SQD	C12-C13-C14-C15
28	D	413	LHG	C18-C19-C20-C21
28	D	413	LHG	C24-C25-C26-C27
28	L	102	LHG	C12-C13-C14-C15
29	A	413	DGD	C4B-C5B-C6B-C7B
29	C	516	DGD	CCB-CDB-CEB-CFB
29	C	517	DGD	C5A-C6A-C7A-C8A
29	C	517	DGD	O6E-C1E-O5D-C6D
30	B	616	BCR	C6-C7-C8-C9
26	d	410	LMG	C34-C35-C36-C37
29	H	103	DGD	C7A-C8A-C9A-CAA
31	M	104	STE	C13-C14-C15-C16
31	X	101	STE	C10-C11-C12-C13
31	b	624	STE	C6-C7-C8-C9
22	c	505	CLA	C5-C6-C7-C8
26	A	409	LMG	C11-C12-C13-C14
31	B	623	STE	C5-C6-C7-C8
31	j	101	STE	C4-C5-C6-C7
26	b	622	LMG	C19-C20-C21-C22
26	c	520	LMG	C35-C36-C37-C38
28	l	101	LHG	C11-C12-C13-C14
27	D	409	SQD	C26-C27-C28-C29
29	C	517	DGD	C8B-C9B-CAB-CBB
31	M	102	STE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
22	b	601	CLA	C16-C17-C18-C19
22	c	503	CLA	C16-C17-C18-C19
28	A	411	LHG	C15-C16-C17-C18
27	a	410	SQD	C8-C7-O47-C45
27	a	410	SQD	C24-C25-C26-C27
29	A	413	DGD	C6B-C7B-C8B-C9B
22	c	504	CLA	C10-C11-C12-C13
26	a	414	LMG	O9-C10-O7-C8
28	D	410	LHG	O9-C7-O7-C5
26	c	520	LMG	C16-C17-C18-C19
28	l	101	LHG	C32-C33-C34-C35
31	b	625	STE	C5-C6-C7-C8
31	d	411	STE	C5-C6-C7-C8
22	b	614	CLA	O1A-CGA-O2A-C1
22	b	610	CLA	C13-C15-C16-C17
30	x	101	BCR	C36-C18-C19-C20
29	H	103	DGD	C4B-C5B-C6B-C7B
27	A	410	SQD	C23-C24-C25-C26
25	A	408	PL9	C22-C23-C24-C25
31	H	104	STE	C2-C3-C4-C5
28	D	411	LHG	C27-C28-C29-C30
28	D	413	LHG	C17-C18-C19-C20
29	c	516	DGD	CBA-CCA-CDA-CEA
22	B	605	CLA	C16-C17-C18-C19
26	a	414	LMG	C35-C36-C37-C38
31	b	628	STE	C6-C7-C8-C9
31	b	629	STE	C2-C3-C4-C5
27	f	102	SQD	C25-C26-C27-C28
29	A	413	DGD	CCA-CDA-CEA-CFA
29	h	101	DGD	C9A-CAA-CBA-CCA
22	a	402	CLA	C15-C16-C17-C18
22	c	503	CLA	C5-C6-C7-C8
27	t	102	SQD	C12-C13-C14-C15
28	b	623	LHG	C15-C16-C17-C18
31	b	626	STE	C12-C13-C14-C15
31	H	104	STE	C13-C14-C15-C16
31	J	101	STE	C2-C3-C4-C5
22	A	405	CLA	C3-C5-C6-C7
22	b	606	CLA	C3-C5-C6-C7
22	C	511	CLA	C8-C10-C11-C12
23	A	404	PHO	C15-C16-C17-C18
31	J	101	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	M	102	STE	C1-C2-C3-C4
26	c	520	LMG	C33-C34-C35-C36
28	a	411	LHG	C11-C10-C9-C8
29	c	516	DGD	C4A-C5A-C6A-C7A
29	c	516	DGD	C7B-C8B-C9B-CAB
31	k	104	STE	C6-C7-C8-C9
25	d	407	PL9	C34-C36-C37-C38
22	B	611	CLA	C10-C11-C12-C13
22	H	101	CLA	C13-C15-C16-C17
22	c	508	CLA	C8-C10-C11-C12
22	B	612	CLA	C16-C17-C18-C19
26	D	408	LMG	C36-C37-C38-C39
27	a	410	SQD	C11-C10-C9-C8
31	Z	101	STE	C11-C12-C13-C14
26	Y	101	LMG	C37-C38-C39-C40
28	b	623	LHG	C11-C10-C9-C8
28	l	101	LHG	C17-C18-C19-C20
28	b	623	LHG	C23-C24-C25-C26
29	C	518	DGD	C1A-C2A-C3A-C4A
22	C	508	CLA	C10-C11-C12-C13
26	a	414	LMG	C38-C39-C40-C41
26	b	622	LMG	C30-C31-C32-C33
26	m	101	LMG	C39-C40-C41-C42
27	f	102	SQD	C28-C29-C30-C31
29	c	515	DGD	CBA-CCA-CDA-CEA
26	a	414	LMG	O7-C8-C9-O8
27	A	410	SQD	O6-C44-C45-O47
27	a	410	SQD	O6-C44-C45-O47
26	A	409	LMG	C35-C36-C37-C38
26	M	101	LMG	C38-C39-C40-C41
26	b	622	LMG	C31-C32-C33-C34
28	l	101	LHG	C24-C25-C26-C27
29	C	517	DGD	C6B-C7B-C8B-C9B
26	a	414	LMG	C30-C31-C32-C33
26	c	521	LMG	C12-C13-C14-C15
28	D	411	LHG	C14-C15-C16-C17
29	H	103	DGD	CBB-CCB-CDB-CEB
31	B	623	STE	C11-C10-C9-C8
31	X	101	STE	C9-C10-C11-C12
26	a	414	LMG	O6-C5-C6-O5
26	a	414	LMG	C17-C18-C19-C20
26	b	622	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
26	c	521	LMG	C31-C32-C33-C34
26	m	101	LMG	C33-C34-C35-C36
28	A	411	LHG	C25-C26-C27-C28
28	a	411	LHG	C17-C18-C19-C20
28	d	408	LHG	C32-C33-C34-C35
29	C	518	DGD	CCB-CDB-CEB-CFB
29	H	103	DGD	C6B-C7B-C8B-C9B
29	h	101	DGD	C6B-C7B-C8B-C9B
28	A	411	LHG	C13-C14-C15-C16
29	c	516	DGD	C6A-C7A-C8A-C9A
31	B	623	STE	C3-C4-C5-C6
31	x	102	STE	C13-C14-C15-C16
22	b	613	CLA	C16-C17-C18-C20
28	L	102	LHG	C28-C29-C30-C31
28	L	102	LHG	C33-C34-C35-C36
28	d	409	LHG	C29-C30-C31-C32
31	B	619	STE	C11-C12-C13-C14
22	C	506	CLA	C4-C3-C5-C6
25	d	407	PL9	C15-C14-C16-C17
28	L	102	LHG	O9-C7-O7-C5
26	A	409	LMG	C13-C14-C15-C16
26	A	409	LMG	C18-C19-C20-C21
26	M	101	LMG	C30-C31-C32-C33
28	L	102	LHG	C15-C16-C17-C18
29	C	516	DGD	C3B-C4B-C5B-C6B
22	c	507	CLA	CBD-CGD-O2D-CED
25	D	407	PL9	C37-C38-C39-C40
26	d	410	LMG	O6-C5-C6-O5
26	B	620	LMG	C29-C30-C31-C32
28	A	411	LHG	C16-C17-C18-C19
28	D	413	LHG	C16-C17-C18-C19
31	B	619	STE	C11-C10-C9-C8
22	C	506	CLA	O1D-CGD-O2D-CED
26	D	412	LMG	C13-C14-C15-C16
26	D	412	LMG	C31-C32-C33-C34
31	B	624	STE	C7-C8-C9-C10
22	B	615	CLA	C5-C6-C7-C8
22	b	615	CLA	C15-C16-C17-C18
26	b	622	LMG	O6-C5-C6-O5
26	b	622	LMG	C10-C11-C12-C13
29	A	413	DGD	CAA-CBA-CCA-CDA
29	C	516	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
27	f	102	SQD	C31-C32-C33-C34
31	b	625	STE	C7-C8-C9-C10
31	b	629	STE	C9-C10-C11-C12
28	A	411	LHG	O1-C1-C2-O2
28	b	623	LHG	O1-C1-C2-O2
28	d	409	LHG	O1-C1-C2-O2
27	B	621	SQD	O10-C23-O48-C46
22	c	511	CLA	C3-C5-C6-C7
29	c	517	DGD	C3A-C4A-C5A-C6A
31	c	519	STE	C10-C11-C12-C13
22	H	101	CLA	C1A-C2A-CAA-CBA
22	c	503	CLA	C1A-C2A-CAA-CBA
22	c	508	CLA	C1A-C2A-CAA-CBA
22	B	609	CLA	C8-C10-C11-C12
22	C	513	CLA	C10-C11-C12-C13
29	C	518	DGD	C3B-C4B-C5B-C6B
27	A	412	SQD	C34-C35-C36-C37
28	D	410	LHG	C30-C31-C32-C33
26	c	518	LMG	O6-C5-C6-O5
29	C	518	DGD	C5A-C6A-C7A-C8A
22	A	403	CLA	C6-C7-C8-C10
22	B	601	CLA	C11-C12-C13-C15
22	B	602	CLA	C6-C7-C8-C10
22	B	602	CLA	C11-C12-C13-C15
22	B	604	CLA	C11-C10-C8-C7
22	B	606	CLA	C11-C10-C8-C7
22	B	606	CLA	C11-C12-C13-C15
22	B	610	CLA	C11-C10-C8-C7
22	B	613	CLA	C11-C12-C13-C15
22	B	613	CLA	C12-C13-C15-C16
22	B	614	CLA	C11-C12-C13-C15
22	B	615	CLA	C6-C7-C8-C10
22	C	504	CLA	C11-C10-C8-C7
22	C	506	CLA	C12-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C7
22	C	511	CLA	C6-C7-C8-C10
22	C	512	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C12-C13-C15
22	a	403	CLA	C11-C10-C8-C7
22	b	604	CLA	C12-C13-C15-C16
22	b	605	CLA	C11-C12-C13-C15
22	b	606	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	b	607	CLA	C6-C7-C8-C10
22	b	609	CLA	C11-C12-C13-C15
22	b	616	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C12-C13-C15
22	c	508	CLA	C11-C10-C8-C7
22	c	508	CLA	C12-C13-C15-C16
22	c	510	CLA	C12-C13-C15-C16
22	c	512	CLA	C6-C7-C8-C10
26	c	521	LMG	C13-C14-C15-C16
31	a	412	STE	C6-C7-C8-C9
22	D	405	CLA	C16-C17-C18-C20
28	l	101	LHG	C30-C31-C32-C33
31	a	413	STE	C11-C12-C13-C14
29	A	413	DGD	C5A-C6A-C7A-C8A
22	C	512	CLA	C15-C16-C17-C18
26	m	101	LMG	C18-C19-C20-C21
22	B	610	CLA	C4-C3-C5-C6
22	C	506	CLA	C2-C3-C5-C6
26	Y	101	LMG	C11-C12-C13-C14
31	b	628	STE	C7-C8-C9-C10
22	C	507	CLA	C10-C11-C12-C13
22	B	611	CLA	C3-C5-C6-C7
27	A	410	SQD	C8-C7-O47-C45
22	A	403	CLA	C6-C7-C8-C9
22	B	601	CLA	C11-C12-C13-C14
22	B	606	CLA	C11-C10-C8-C9
22	B	614	CLA	C11-C12-C13-C14
22	C	504	CLA	C11-C10-C8-C9
22	C	511	CLA	C6-C7-C8-C9
22	D	405	CLA	C6-C7-C8-C9
22	a	403	CLA	C11-C10-C8-C9
22	b	601	CLA	C11-C12-C13-C14
22	b	604	CLA	C14-C13-C15-C16
22	b	606	CLA	C14-C13-C15-C16
22	b	607	CLA	C11-C12-C13-C14
22	c	506	CLA	C11-C10-C8-C9
22	c	506	CLA	C11-C12-C13-C14
22	c	508	CLA	C11-C10-C8-C9
22	c	510	CLA	C14-C13-C15-C16
22	c	512	CLA	C14-C13-C15-C16
22	d	403	CLA	C6-C7-C8-C9
26	a	414	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
28	D	413	LHG	C31-C32-C33-C34
22	c	512	CLA	C8-C10-C11-C12
22	C	508	CLA	C13-C15-C16-C17
28	D	413	LHG	C13-C14-C15-C16
26	Y	101	LMG	O1-C7-C8-C9
26	c	520	LMG	O1-C7-C8-C9
26	c	520	LMG	C7-C8-C9-O8
26	c	521	LMG	O1-C7-C8-C9
27	B	621	SQD	O6-C44-C45-C46
29	A	413	DGD	C1G-C2G-C3G-O3G
29	C	516	DGD	O1G-C1G-C2G-C3G
31	d	411	STE	C2-C3-C4-C5
22	H	101	CLA	C3-C5-C6-C7
26	b	622	LMG	C18-C19-C20-C21
22	b	601	CLA	C10-C11-C12-C13
26	b	622	LMG	C16-C17-C18-C19
29	C	518	DGD	C6A-C7A-C8A-C9A
22	C	509	CLA	C16-C17-C18-C19
29	A	413	DGD	C7A-C8A-C9A-CAA
29	h	101	DGD	C3B-C4B-C5B-C6B
31	C	519	STE	C2-C3-C4-C5
27	a	410	SQD	C25-C26-C27-C28
29	c	515	DGD	O6E-C5E-C6E-O5E
26	c	521	LMG	C36-C37-C38-C39
26	m	101	LMG	C12-C13-C14-C15
30	b	618	BCR	C16-C17-C18-C36
22	B	607	CLA	C10-C11-C12-C13
28	D	410	LHG	C13-C14-C15-C16
27	D	409	SQD	C27-C28-C29-C30
22	B	610	CLA	C2-C3-C5-C6
22	b	611	CLA	C2-C3-C5-C6
22	c	505	CLA	C2-C3-C5-C6
25	d	407	PL9	C13-C14-C16-C17
25	d	407	PL9	C28-C29-C31-C32
25	d	407	PL9	C33-C34-C36-C37
27	A	412	SQD	C9-C10-C11-C12
22	B	613	CLA	C15-C16-C17-C18
22	b	602	CLA	C15-C16-C17-C18
22	C	502	CLA	C16-C17-C18-C19
28	a	411	LHG	C25-C26-C27-C28
29	C	517	DGD	C2B-C3B-C4B-C5B
31	b	629	STE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	D	408	LMG	O6-C5-C6-O5
22	C	507	CLA	C5-C6-C7-C8
22	C	510	CLA	C8-C10-C11-C12
31	a	412	STE	C2-C3-C4-C5
26	a	414	LMG	C23-C24-C25-C26
26	b	622	LMG	C38-C39-C40-C41
27	a	410	SQD	C13-C14-C15-C16
31	b	627	STE	C4-C5-C6-C7
27	A	412	SQD	C16-C17-C18-C19
29	H	103	DGD	C8B-C9B-CAB-CBB
29	c	516	DGD	C2B-C3B-C4B-C5B
31	X	101	STE	C14-C15-C16-C17
31	c	519	STE	C7-C8-C9-C10
22	C	510	CLA	O1D-CGD-O2D-CED
22	c	501	CLA	O1D-CGD-O2D-CED
22	B	604	CLA	CBA-CGA-O2A-C1
22	b	607	CLA	CBA-CGA-O2A-C1
26	D	412	LMG	C29-C28-O8-C9
27	A	412	SQD	C24-C23-O48-C46
22	D	405	CLA	O2A-C1-C2-C3
26	b	622	LMG	C34-C35-C36-C37
27	L	101	SQD	C9-C10-C11-C12
28	D	413	LHG	C25-C26-C27-C28
29	c	515	DGD	CAB-CBB-CCB-CDB
29	c	517	DGD	CCA-CDA-CEA-CFA
31	H	104	STE	C5-C6-C7-C8
30	B	617	BCR	C18-C19-C20-C21
22	B	601	CLA	C8-C10-C11-C12
29	c	517	DGD	C2A-C3A-C4A-C5A
31	X	101	STE	C3-C4-C5-C6
30	k	102	BCR	C19-C20-C21-C22
22	D	405	CLA	C16-C17-C18-C19
22	d	403	CLA	C16-C17-C18-C20
27	A	410	SQD	C11-C10-C9-C8
27	A	412	SQD	C15-C16-C17-C18
22	b	602	CLA	O1D-CGD-O2D-CED
30	d	406	BCR	C16-C17-C18-C19
26	Y	101	LMG	C33-C34-C35-C36
27	A	412	SQD	C11-C10-C9-C8
27	t	102	SQD	C24-C23-O48-C46
31	k	104	STE	C7-C8-C9-C10
27	A	412	SQD	C44-C45-O47-C7

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Mol	Chain	Res	Type	Atoms
26	D	408	LMG	C15-C16-C17-C18
26	c	521	LMG	C33-C34-C35-C36
26	Y	101	LMG	C15-C16-C17-C18
31	c	519	STE	C4-C5-C6-C7
22	c	505	CLA	C4-C3-C5-C6
22	C	510	CLA	C2-C3-C5-C6
26	d	410	LMG	C15-C16-C17-C18
26	D	412	LMG	C36-C37-C38-C39
27	A	412	SQD	C28-C29-C30-C31
27	L	101	SQD	C26-C27-C28-C29
22	b	607	CLA	C16-C17-C18-C20
26	Y	101	LMG	C14-C15-C16-C17
26	m	101	LMG	C15-C16-C17-C18
28	D	411	LHG	C30-C31-C32-C33
29	C	517	DGD	C4A-C5A-C6A-C7A
29	c	516	DGD	CAB-CBB-CCB-CDB
26	D	412	LMG	C12-C13-C14-C15
31	R	101	STE	C4-C5-C6-C7
27	a	410	SQD	O47-C45-C46-O48
31	b	621	STE	C6-C7-C8-C9
22	C	506	CLA	CBA-CGA-O2A-C1
29	C	517	DGD	CDA-CEA-CFA-CGA
31	b	629	STE	C15-C16-C17-C18
26	D	412	LMG	C37-C38-C39-C40
31	a	413	STE	C13-C14-C15-C16
31	b	620	STE	C3-C4-C5-C6
31	b	627	STE	C7-C8-C9-C10
26	b	622	LMG	C15-C16-C17-C18
27	B	621	SQD	C32-C33-C34-C35
28	D	413	LHG	C32-C33-C34-C35
28	d	408	LHG	C11-C10-C9-C8
22	C	509	CLA	C3-C5-C6-C7
31	b	624	STE	C7-C8-C9-C10
27	L	101	SQD	C19-C20-C21-C22
26	d	410	LMG	C30-C31-C32-C33
31	b	625	STE	C10-C11-C12-C13
29	c	515	DGD	CBB-CCB-CDB-CEB
31	X	101	STE	C6-C7-C8-C9
26	A	409	LMG	C37-C38-C39-C40
26	D	412	LMG	C34-C35-C36-C37
27	B	621	SQD	C13-C14-C15-C16
27	L	101	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
29	c	515	DGD	C5B-C6B-C7B-C8B
31	C	520	STE	C11-C10-C9-C8
31	R	101	STE	C3-C4-C5-C6
31	k	104	STE	C4-C5-C6-C7
22	a	405	CLA	CBA-CGA-O2A-C1
31	L	103	STE	C6-C7-C8-C9
31	t	104	STE	C7-C8-C9-C10
22	C	513	CLA	C8-C10-C11-C12
22	B	607	CLA	C16-C17-C18-C20
22	C	509	CLA	C16-C17-C18-C20
22	b	609	CLA	C16-C17-C18-C19
22	b	611	CLA	C4-C3-C5-C6
25	A	408	PL9	C15-C14-C16-C17
25	D	407	PL9	C30-C29-C31-C32
25	d	407	PL9	C45-C44-C46-C47
25	D	407	PL9	C28-C29-C31-C32
22	C	511	CLA	CBA-CGA-O2A-C1
29	A	413	DGD	CEB-CFB-CGB-CHB
28	A	411	LHG	C18-C19-C20-C21
27	D	409	SQD	C45-C44-O6-C1
22	B	602	CLA	C6-C7-C8-C9
22	B	602	CLA	C11-C12-C13-C14
22	B	606	CLA	C11-C12-C13-C14
22	B	615	CLA	C6-C7-C8-C9
22	C	506	CLA	C6-C7-C8-C9
22	C	506	CLA	C14-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C9
22	C	512	CLA	C11-C12-C13-C14
22	C	513	CLA	C11-C10-C8-C9
22	D	404	CLA	C11-C12-C13-C14
22	D	405	CLA	C11-C10-C8-C9
22	b	603	CLA	C6-C7-C8-C9
22	b	605	CLA	C11-C12-C13-C14
22	b	607	CLA	C6-C7-C8-C9
22	b	607	CLA	C14-C13-C15-C16
31	J	101	STE	C3-C4-C5-C6
31	c	519	STE	C11-C12-C13-C14
22	B	605	CLA	C5-C6-C7-C8
22	B	612	CLA	C5-C6-C7-C8
22	b	611	CLA	C13-C15-C16-C17
22	b	602	CLA	C4B-C3B-CAB-CBB
29	c	517	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
28	b	623	LHG	C19-C20-C21-C22
29	c	516	DGD	CBB-CCB-CDB-CEB
22	c	513	CLA	C5-C6-C7-C8
22	B	609	CLA	C16-C17-C18-C19
22	B	610	CLA	C16-C17-C18-C19
29	H	103	DGD	C5B-C6B-C7B-C8B
29	C	517	DGD	CAA-CBA-CCA-CDA
31	a	412	STE	C3-C4-C5-C6
26	c	521	LMG	C2-C1-O1-C7
26	Y	101	LMG	C32-C33-C34-C35
26	c	520	LMG	C32-C33-C34-C35
27	A	410	SQD	C29-C30-C31-C32
27	D	409	SQD	C28-C29-C30-C31
27	a	410	SQD	C32-C33-C34-C35
28	d	408	LHG	C34-C35-C36-C37
31	B	623	STE	C12-C13-C14-C15
31	a	413	STE	C10-C11-C12-C13
27	A	410	SQD	C17-C18-C19-C20
27	t	102	SQD	C10-C11-C12-C13
28	D	411	LHG	C13-C14-C15-C16
29	C	516	DGD	O1G-C1A-C2A-C3A
22	B	603	CLA	C12-C13-C15-C16
22	B	605	CLA	C11-C10-C8-C7
22	B	606	CLA	C12-C13-C15-C16
22	C	502	CLA	C12-C13-C15-C16
22	C	503	CLA	C11-C10-C8-C7
22	C	506	CLA	C6-C7-C8-C10
22	C	509	CLA	C12-C13-C15-C16
22	C	513	CLA	C11-C10-C8-C7
22	D	403	CLA	C11-C12-C13-C15
22	D	404	CLA	C11-C12-C13-C15
22	D	405	CLA	C6-C7-C8-C10
22	D	405	CLA	C11-C10-C8-C7
22	D	405	CLA	C11-C12-C13-C15
22	a	403	CLA	C12-C13-C15-C16
22	b	601	CLA	C11-C12-C13-C15
22	b	603	CLA	C6-C7-C8-C10
22	b	607	CLA	C11-C12-C13-C15
22	b	608	CLA	C11-C10-C8-C7
22	b	615	CLA	C11-C10-C8-C7
22	c	501	CLA	C11-C12-C13-C15
22	c	506	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	c	509	CLA	C6-C7-C8-C10
22	c	512	CLA	C12-C13-C15-C16
22	d	403	CLA	C6-C7-C8-C10
22	b	605	CLA	C13-C15-C16-C17
22	c	502	CLA	C15-C16-C17-C18
26	c	521	LMG	C20-C21-C22-C23
31	a	412	STE	C7-C8-C9-C10
27	B	621	SQD	C7-C8-C9-C10
26	B	620	LMG	C37-C38-C39-C40
31	b	620	STE	C15-C16-C17-C18
31	M	102	STE	C4-C5-C6-C7
31	Z	101	STE	C12-C13-C14-C15
22	C	506	CLA	C3A-C2A-CAA-CBA
22	C	510	CLA	C4-C3-C5-C6
22	b	601	CLA	C3A-C2A-CAA-CBA
22	C	506	CLA	C10-C11-C12-C13
27	a	410	SQD	C14-C15-C16-C17
25	d	407	PL9	C43-C44-C46-C47
29	H	103	DGD	CDB-CEB-CFB-CGB
28	l	101	LHG	C25-C26-C27-C28
26	D	408	LMG	C35-C36-C37-C38
29	c	517	DGD	C8B-C9B-CAB-CBB
22	b	607	CLA	O1A-CGA-O2A-C1
31	b	624	STE	C4-C5-C6-C7
26	Y	101	LMG	C29-C28-O8-C9
26	c	521	LMG	C39-C40-C41-C42
28	l	101	LHG	C34-C35-C36-C37
30	H	102	BCR	C13-C14-C15-C16
30	H	102	BCR	C15-C16-C17-C18
22	B	606	CLA	C16-C17-C18-C19
26	D	412	LMG	C16-C17-C18-C19
26	c	521	LMG	C35-C36-C37-C38
28	D	411	LHG	C29-C30-C31-C32
29	h	101	DGD	CAB-CBB-CCB-CDB
31	M	104	STE	C3-C4-C5-C6
22	B	606	CLA	C10-C11-C12-C13
22	c	503	CLA	C15-C16-C17-C18
22	c	509	CLA	C13-C15-C16-C17
26	Y	101	LMG	C12-C13-C14-C15
27	a	410	SQD	C16-C17-C18-C19
31	B	619	STE	C9-C10-C11-C12
29	h	101	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
28	A	411	LHG	C10-C11-C12-C13
28	D	410	LHG	C25-C26-C27-C28
28	L	102	LHG	C13-C14-C15-C16
26	M	101	LMG	C7-C8-C9-O8
26	a	414	LMG	C7-C8-C9-O8
27	A	410	SQD	O6-C44-C45-C46
27	L	101	SQD	C44-C45-C46-O48
27	a	410	SQD	O6-C44-C45-C46
27	f	102	SQD	C29-C30-C31-C32
22	B	607	CLA	C16-C17-C18-C19
22	b	609	CLA	C16-C17-C18-C20
28	a	411	LHG	C14-C15-C16-C17
29	c	515	DGD	C6B-C7B-C8B-C9B
26	D	412	LMG	O1-C7-C8-C9
29	A	413	DGD	C7B-C8B-C9B-CAB
22	b	604	CLA	C3-C5-C6-C7
22	B	607	CLA	C5-C6-C7-C8
23	A	404	PHO	C10-C11-C12-C13
22	B	603	CLA	O1D-CGD-O2D-CED
26	c	521	LMG	C19-C20-C21-C22
29	c	515	DGD	C3A-C4A-C5A-C6A
22	b	615	CLA	C16-C17-C18-C19
30	T	101	BCR	C5-C6-C7-C8
30	k	102	BCR	C23-C24-C25-C30
30	x	101	BCR	C23-C24-C25-C30
26	a	414	LMG	C37-C38-C39-C40
28	D	410	LHG	C11-C10-C9-C8
29	H	103	DGD	CCA-CDA-CEA-CFA
22	D	405	CLA	CBD-CGD-O2D-CED
27	L	101	SQD	C16-C17-C18-C19
29	h	101	DGD	C7B-C8B-C9B-CAB
28	b	623	LHG	C29-C30-C31-C32
22	B	606	CLA	C16-C17-C18-C20
22	c	509	CLA	CAA-CBA-CGA-O2A
22	D	404	CLA	C15-C16-C17-C18
26	Y	101	LMG	O1-C7-C8-O7
26	c	520	LMG	O1-C7-C8-O7
29	A	413	DGD	O1G-C1G-C2G-O2G
28	L	102	LHG	O10-C23-O8-C6
25	D	407	PL9	C4-C3-C7-C8
25	a	409	PL9	C4-C3-C7-C8
31	b	621	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	A	403	CLA	C3-C5-C6-C7
27	B	621	SQD	C29-C30-C31-C32
29	c	517	DGD	C7B-C8B-C9B-CAB
22	C	505	CLA	C4-C3-C5-C6
28	D	413	LHG	C27-C28-C29-C30
25	D	407	PL9	C13-C14-C16-C17
26	D	408	LMG	C37-C38-C39-C40
27	A	412	SQD	C13-C14-C15-C16
22	C	502	CLA	C16-C17-C18-C20
26	a	414	LMG	C32-C33-C34-C35
27	D	409	SQD	O6-C44-C45-C46
28	b	623	LHG	C7-C8-C9-C10
31	t	104	STE	C3-C4-C5-C6
28	a	411	LHG	C8-C7-O7-C5
22	B	604	CLA	C11-C10-C8-C9
22	H	101	CLA	C11-C10-C8-C9
22	b	615	CLA	C11-C10-C8-C9
27	a	410	SQD	C30-C31-C32-C33
31	B	619	STE	C4-C5-C6-C7
22	C	511	CLA	O1A-CGA-O2A-C1
26	b	622	LMG	C29-C30-C31-C32
26	D	408	LMG	C40-C41-C42-C43
26	a	414	LMG	C24-C25-C26-C27
26	c	521	LMG	O6-C5-C6-O5
22	b	612	CLA	C10-C11-C12-C13
26	D	412	LMG	O1-C7-C8-O7
31	k	104	STE	C2-C3-C4-C5
23	D	401	PHO	C13-C15-C16-C17
29	c	515	DGD	CDB-CEB-CFB-CGB
28	D	410	LHG	O2-C2-C3-O3
22	c	506	CLA	CBA-CGA-O2A-C1
22	d	403	CLA	C16-C17-C18-C19
26	a	414	LMG	C16-C17-C18-C19
26	A	409	LMG	C14-C15-C16-C17
27	B	621	SQD	C25-C26-C27-C28
31	B	624	STE	C11-C10-C9-C8
31	b	627	STE	C3-C4-C5-C6
27	B	621	SQD	C24-C25-C26-C27
30	B	617	BCR	C20-C21-C22-C37
30	C	514	BCR	C35-C13-C14-C15
30	c	514	BCR	C20-C21-C22-C37
27	a	410	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
27	A	410	SQD	C28-C29-C30-C31
29	H	103	DGD	C3B-C4B-C5B-C6B
28	l	101	LHG	O6-C4-C5-C6
22	B	610	CLA	C16-C17-C18-C20
22	b	602	CLA	C16-C17-C18-C19
29	C	516	DGD	C9A-CAA-CBA-CCA
30	b	618	BCR	C37-C22-C23-C24
27	A	412	SQD	C18-C19-C20-C21
22	A	403	CLA	C11-C12-C13-C15
22	B	603	CLA	C11-C12-C13-C15
22	H	101	CLA	C11-C10-C8-C7
22	b	605	CLA	C11-C10-C8-C7
22	c	511	CLA	C11-C12-C13-C15
23	A	404	PHO	C12-C13-C15-C16
29	h	101	DGD	C1A-C2A-C3A-C4A
29	C	517	DGD	C4B-C5B-C6B-C7B
22	b	610	CLA	O1D-CGD-O2D-CED
31	b	626	STE	C10-C11-C12-C13
30	C	515	BCR	C7-C8-C9-C10
30	K	101	BCR	C11-C12-C13-C14
30	k	101	BCR	C21-C22-C23-C24
31	H	104	STE	C11-C10-C9-C8
22	B	604	CLA	O1A-CGA-O2A-C1
29	C	517	DGD	C2G-C3G-O3G-C1D
29	C	517	DGD	C5D-C6D-O5D-C1E
29	c	516	DGD	C2G-C3G-O3G-C1D
22	c	511	CLA	C2C-C3C-CAC-CBC
28	D	410	LHG	C23-C24-C25-C26
22	c	501	CLA	C2A-CAA-CBA-CGA
26	m	101	LMG	C16-C17-C18-C19
28	d	408	LHG	C16-C17-C18-C19
31	I	102	STE	C11-C10-C9-C8
22	B	602	CLA	C16-C17-C18-C19
29	C	518	DGD	C3A-C4A-C5A-C6A
22	a	405	CLA	O1A-CGA-O2A-C1
22	c	506	CLA	O1A-CGA-O2A-C1
29	C	517	DGD	O1A-C1A-O1G-C1G
23	A	404	PHO	C2-C3-C5-C6
26	a	414	LMG	C34-C35-C36-C37
28	L	102	LHG	C35-C36-C37-C38
31	B	625	STE	C7-C8-C9-C10
31	b	627	STE	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
28	D	410	LHG	C12-C13-C14-C15
27	f	102	SQD	C46-C45-O47-C7
22	C	506	CLA	O1A-CGA-O2A-C1
28	L	102	LHG	C17-C18-C19-C20
23	d	401	PHO	CBD-CGD-O2D-CED
31	b	628	STE	C12-C13-C14-C15
22	B	604	CLA	C16-C17-C18-C20
28	d	409	LHG	C35-C36-C37-C38
31	Z	101	STE	C14-C15-C16-C17
22	B	609	CLA	C15-C16-C17-C18
22	b	609	CLA	C15-C16-C17-C18
30	B	617	BCR	C12-C13-C14-C15
30	B	618	BCR	C12-C13-C14-C15
30	c	514	BCR	C11-C10-C9-C8
31	H	104	STE	C6-C7-C8-C9
27	A	412	SQD	C29-C30-C31-C32
28	L	102	LHG	C18-C19-C20-C21
29	A	413	DGD	O1G-C1G-C2G-C3G
31	x	102	STE	C15-C16-C17-C18
22	c	502	CLA	CBD-CGD-O2D-CED
22	B	606	CLA	C15-C16-C17-C18
22	b	601	CLA	C8-C10-C11-C12
22	B	614	CLA	C16-C17-C18-C19
22	C	508	CLA	C16-C17-C18-C19
29	A	413	DGD	C4A-C5A-C6A-C7A
22	B	614	CLA	C5-C6-C7-C8
31	I	102	STE	C2-C3-C4-C5
22	C	505	CLA	C2-C3-C5-C6
28	L	102	LHG	C32-C33-C34-C35
28	a	411	LHG	C26-C27-C28-C29
29	C	517	DGD	CBB-CCB-CDB-CEB
26	D	412	LMG	C11-C12-C13-C14
31	a	413	STE	C2-C3-C4-C5
31	H	104	STE	C10-C11-C12-C13
26	c	520	LMG	O7-C8-C9-O8
26	c	521	LMG	O1-C7-C8-O7
22	A	403	CLA	C11-C12-C13-C14
22	d	405	CLA	C6-C7-C8-C9
27	A	410	SQD	C11-C12-C13-C14
27	A	410	SQD	C26-C27-C28-C29
31	x	102	STE	C11-C10-C9-C8
27	A	410	SQD	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	H	103	DGD	CAB-CBB-CCB-CDB
31	b	621	STE	C2-C3-C4-C5
31	b	621	STE	C11-C10-C9-C8
22	b	604	CLA	C15-C16-C17-C18
26	D	408	LMG	C20-C21-C22-C23
26	m	101	LMG	C32-C33-C34-C35
28	A	411	LHG	C31-C32-C33-C34
31	b	621	STE	C10-C11-C12-C13
31	b	625	STE	C12-C13-C14-C15
31	B	624	STE	C10-C11-C12-C13
22	d	404	CLA	C13-C15-C16-C17
31	L	103	STE	C7-C8-C9-C10
29	H	103	DGD	O2G-C1B-C2B-C3B
27	A	410	SQD	C15-C16-C17-C18
27	f	102	SQD	C33-C34-C35-C36
31	M	104	STE	C12-C13-C14-C15
28	d	408	LHG	C15-C16-C17-C18
27	a	410	SQD	C35-C36-C37-C38
28	D	411	LHG	C11-C10-C9-C8
31	M	102	STE	C11-C10-C9-C8
31	t	103	STE	C6-C7-C8-C9
22	c	507	CLA	C4-C3-C5-C6
23	A	404	PHO	C4-C3-C5-C6
25	d	407	PL9	C30-C29-C31-C32
31	B	624	STE	C14-C15-C16-C17
22	b	610	CLA	C2A-CAA-CBA-CGA
22	C	508	CLA	CBD-CGD-O2D-CED
29	H	103	DGD	CBA-CCA-CDA-CEA
22	B	614	CLA	C16-C17-C18-C20
22	D	403	CLA	C16-C17-C18-C19
22	b	602	CLA	C16-C17-C18-C20
26	D	408	LMG	C31-C32-C33-C34
27	L	101	SQD	C18-C19-C20-C21
31	B	619	STE	C2-C3-C4-C5
28	D	413	LHG	C7-C8-C9-C10
26	Y	101	LMG	C17-C18-C19-C20
27	a	410	SQD	C27-C28-C29-C30
27	B	621	SQD	C9-C10-C11-C12
26	b	622	LMG	C32-C33-C34-C35
22	B	602	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C20
34	V	201	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	t	102	SQD	C14-C15-C16-C17
22	H	101	CLA	C4B-C3B-CAB-CBB
22	a	405	CLA	C1A-C2A-CAA-CBA
26	M	101	LMG	C19-C20-C21-C22
29	H	103	DGD	CCB-CDB-CEB-CFB
27	D	409	SQD	O48-C23-C24-C25
28	D	410	LHG	C32-C33-C34-C35
31	M	103	STE	C2-C3-C4-C5
29	c	515	DGD	C4D-C5D-C6D-O5D
27	L	101	SQD	C23-C24-C25-C26
31	X	101	STE	C7-C8-C9-C10
28	a	411	LHG	O6-C4-C5-C6
29	C	516	DGD	O1B-C1B-O2G-C2G
31	C	520	STE	C4-C5-C6-C7
31	M	104	STE	C9-C10-C11-C12
22	B	604	CLA	C6-C7-C8-C10
22	B	612	CLA	C12-C13-C15-C16
22	a	403	CLA	C11-C12-C13-C15
22	b	601	CLA	C11-C10-C8-C7
22	b	606	CLA	C11-C12-C13-C15
22	b	612	CLA	C12-C13-C15-C16
22	c	505	CLA	C6-C7-C8-C10
22	d	405	CLA	C11-C12-C13-C15
31	M	104	STE	C5-C6-C7-C8
22	b	607	CLA	C16-C17-C18-C19
28	b	623	LHG	C33-C34-C35-C36
29	h	101	DGD	C7A-C8A-C9A-CAA
22	C	511	CLA	CBD-CGD-O2D-CED
26	b	622	LMG	C35-C36-C37-C38
28	l	101	LHG	C18-C19-C20-C21
27	A	412	SQD	C27-C28-C29-C30
27	L	101	SQD	C30-C31-C32-C33
22	b	601	CLA	C5-C6-C7-C8
22	B	601	CLA	C16-C17-C18-C19
26	D	412	LMG	C33-C34-C35-C36
28	D	411	LHG	C15-C16-C17-C18
22	b	616	CLA	C8-C10-C11-C12
26	b	622	LMG	C42-C43-C44-C45
31	I	102	STE	C12-C13-C14-C15
25	D	407	PL9	C2-C3-C7-C8
28	l	101	LHG	O6-C4-C5-O7
22	B	603	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	D	403	CLA	C11-C12-C13-C14
22	b	606	CLA	C6-C7-C8-C9
22	b	613	CLA	C11-C10-C8-C9
22	c	501	CLA	C11-C12-C13-C14
22	c	511	CLA	C11-C12-C13-C14
26	a	414	LMG	C36-C37-C38-C39
28	a	411	LHG	C11-C12-C13-C14
30	c	514	BCR	C13-C14-C15-C16
30	k	101	BCR	C9-C10-C11-C12
28	b	623	LHG	C14-C15-C16-C17
28	l	101	LHG	C14-C15-C16-C17
31	C	520	STE	C6-C7-C8-C9
26	D	408	LMG	C16-C17-C18-C19
26	M	101	LMG	O7-C8-C9-O8
26	a	414	LMG	O1-C7-C8-O7
27	L	101	SQD	O6-C44-C45-O47
27	L	101	SQD	O47-C45-C46-O48
27	t	102	SQD	O47-C45-C46-O48
29	C	516	DGD	O1G-C1G-C2G-O2G
31	b	620	STE	C10-C11-C12-C13
26	D	408	LMG	C33-C34-C35-C36
22	b	610	CLA	C16-C17-C18-C19
26	m	101	LMG	C7-C8-C9-O8
22	B	606	CLA	C13-C15-C16-C17
26	c	520	LMG	C41-C42-C43-C44
31	b	620	STE	C11-C12-C13-C14
29	C	516	DGD	CDA-CEA-CFA-CGA
22	B	606	CLA	CAD-CBD-CGD-O2D
22	B	611	CLA	CAD-CBD-CGD-O2D
22	B	613	CLA	CAD-CBD-CGD-O2D
22	C	506	CLA	CAD-CBD-CGD-O2D
22	H	101	CLA	CAD-CBD-CGD-O2D
22	c	502	CLA	CAD-CBD-CGD-O2D
22	c	506	CLA	CAD-CBD-CGD-O2D
26	B	620	LMG	C36-C37-C38-C39
26	D	412	LMG	C15-C16-C17-C18
31	b	627	STE	C5-C6-C7-C8
26	a	414	LMG	O6-C1-O1-C7
22	B	612	CLA	C13-C15-C16-C17
28	b	623	LHG	C17-C18-C19-C20
26	m	101	LMG	C29-C28-O8-C9
29	C	516	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
22	B	606	CLA	CAD-CBD-CGD-O1D
22	B	611	CLA	CAD-CBD-CGD-O1D
22	B	613	CLA	CAD-CBD-CGD-O1D
22	C	504	CLA	CAD-CBD-CGD-O1D
22	C	506	CLA	CAD-CBD-CGD-O1D
22	H	101	CLA	CAD-CBD-CGD-O1D
22	c	502	CLA	CAD-CBD-CGD-O1D
22	c	506	CLA	CAD-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O2D
23	d	401	PHO	CHA-CBD-CGD-O1D
23	d	401	PHO	CHA-CBD-CGD-O2D
28	A	411	LHG	C4-O6-P-O5
28	L	102	LHG	C4-O6-P-O3
28	b	623	LHG	C3-O3-P-O6
30	t	101	BCR	C13-C14-C15-C16
22	b	603	CLA	C13-C15-C16-C17
22	B	601	CLA	C16-C17-C18-C20
22	c	512	CLA	C10-C11-C12-C13
22	c	512	CLA	C4-C3-C5-C6
22	b	603	CLA	C2B-C3B-CAB-CBB
30	k	102	BCR	C1-C6-C7-C8
28	D	410	LHG	C26-C27-C28-C29
22	c	507	CLA	C2-C3-C5-C6
25	A	408	PL9	C13-C14-C16-C17
22	b	611	CLA	C5-C6-C7-C8
28	b	623	LHG	C2-C3-O3-P
28	d	409	LHG	C2-C3-O3-P
30	I	101	BCR	C7-C8-C9-C34
28	l	101	LHG	C33-C34-C35-C36
28	a	411	LHG	C7-C8-C9-C10
29	C	517	DGD	C3A-C4A-C5A-C6A
28	D	411	LHG	C9-C10-C11-C12
26	d	410	LMG	C12-C13-C14-C15
28	d	409	LHG	C26-C27-C28-C29
29	c	515	DGD	C1A-C2A-C3A-C4A
25	a	409	PL9	C41-C42-C43-C44
25	A	408	PL9	C4-C3-C7-C8
29	A	413	DGD	CFB-CGB-CHB-CIB
29	C	518	DGD	O1A-C1A-O1G-C1G
26	m	101	LMG	C37-C38-C39-C40
27	L	101	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
26	D	412	LMG	C9-C8-O7-C10
28	a	411	LHG	C28-C29-C30-C31
30	C	515	BCR	C9-C10-C11-C12
29	H	103	DGD	C9A-CAA-CBA-CCA
29	c	517	DGD	CAA-CBA-CCA-CDA
22	B	603	CLA	C14-C13-C15-C16
22	B	608	CLA	C14-C13-C15-C16
22	C	509	CLA	C14-C13-C15-C16
22	b	608	CLA	C11-C10-C8-C9
22	c	511	CLA	C11-C10-C8-C9
22	C	509	CLA	C11-C10-C8-C7
22	C	513	CLA	C12-C13-C15-C16
26	D	408	LMG	C21-C22-C23-C24
30	B	618	BCR	C20-C21-C22-C23
30	C	514	BCR	C11-C10-C9-C8
30	b	618	BCR	C12-C13-C14-C15
30	d	406	BCR	C12-C13-C14-C15
26	D	408	LMG	C12-C13-C14-C15
22	c	507	CLA	O1D-CGD-O2D-CED
28	A	411	LHG	C11-C10-C9-C8
31	t	103	STE	C7-C8-C9-C10
26	c	518	LMG	C32-C33-C34-C35
28	A	411	LHG	C17-C18-C19-C20
22	b	601	CLA	C13-C15-C16-C17
29	c	515	DGD	C9B-CAB-CBB-CCB
22	b	604	CLA	C13-C15-C16-C17
28	D	411	LHG	C31-C32-C33-C34
29	C	516	DGD	C2A-C3A-C4A-C5A
23	d	401	PHO	O1D-CGD-O2D-CED
29	c	515	DGD	O6D-C5D-C6D-O5D
31	d	411	STE	C3-C4-C5-C6
26	c	518	LMG	C34-C35-C36-C37
25	A	408	PL9	C19-C21-C22-C23
26	b	622	LMG	O1-C7-C8-C9
28	d	408	LHG	C28-C29-C30-C31
31	b	624	STE	C11-C12-C13-C14
22	A	402	CLA	C15-C16-C17-C18
26	a	414	LMG	C8-C7-O1-C1
22	B	604	CLA	C10-C11-C12-C13
22	c	510	CLA	C15-C16-C17-C18
30	C	515	BCR	C13-C14-C15-C16
30	k	101	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
22	C	508	CLA	C16-C17-C18-C20
28	b	623	LHG	C30-C31-C32-C33
26	b	622	LMG	C28-C29-C30-C31
22	c	502	CLA	O1D-CGD-O2D-CED
22	D	403	CLA	C16-C17-C18-C20
22	a	403	CLA	C14-C13-C15-C16
22	b	615	CLA	C11-C12-C13-C14
31	b	626	STE	C14-C15-C16-C17
22	c	510	CLA	C8-C10-C11-C12
27	B	621	SQD	C31-C32-C33-C34
28	d	409	LHG	C31-C32-C33-C34
22	B	609	CLA	C4B-C3B-CAB-CBB
28	L	102	LHG	C29-C30-C31-C32
23	d	401	PHO	C2C-C3C-CAC-CBC
22	a	405	CLA	C15-C16-C17-C18
31	B	623	STE	C2-C3-C4-C5
31	x	102	STE	C14-C15-C16-C17
31	b	625	STE	C11-C10-C9-C8
22	C	510	CLA	C6-C7-C8-C10
22	C	510	CLA	C12-C13-C15-C16
28	b	623	LHG	C28-C29-C30-C31
22	d	403	CLA	C3-C5-C6-C7
31	t	103	STE	C11-C10-C9-C8
22	b	610	CLA	C16-C17-C18-C20
26	m	101	LMG	O7-C8-C9-O8
22	B	607	CLA	C4-C3-C5-C6
23	D	401	PHO	C3A-C2A-CAA-CBA
27	B	621	SQD	C30-C31-C32-C33
25	a	409	PL9	C43-C44-C46-C47
28	A	411	LHG	C27-C28-C29-C30
28	a	411	LHG	C15-C16-C17-C18
22	A	402	CLA	C13-C15-C16-C17
22	b	614	CLA	C5-C6-C7-C8
28	d	408	LHG	C17-C18-C19-C20
28	D	411	LHG	O9-C7-O7-C5
22	c	513	CLA	C2-C1-O2A-CGA
30	k	103	BCR	C9-C10-C11-C12
30	b	618	BCR	C7-C8-C9-C34
30	k	102	BCR	C36-C18-C19-C20
26	a	414	LMG	O8-C28-C29-C30
29	c	516	DGD	C4E-C5E-C6E-O5E
28	a	411	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	b	612	CLA	C15-C16-C17-C18
29	C	517	DGD	CCB-CDB-CEB-CFB
22	C	501	CLA	C2C-C3C-CAC-CBC
22	B	613	CLA	C13-C15-C16-C17
31	B	623	STE	C11-C12-C13-C14
22	b	615	CLA	C4-C3-C5-C6
29	c	515	DGD	O1G-C1A-C2A-C3A
22	c	512	CLA	C2-C3-C5-C6
22	C	507	CLA	C13-C15-C16-C17
31	d	411	STE	O1-C1-C2-C3
27	a	410	SQD	C44-C45-C46-O48
28	L	102	LHG	C11-C12-C13-C14
30	B	617	BCR	C14-C15-C16-C17
22	B	614	CLA	C13-C15-C16-C17
26	M	101	LMG	C17-C18-C19-C20
31	t	104	STE	C4-C5-C6-C7
31	B	622	STE	O1-C1-C2-C3
22	B	609	CLA	C14-C13-C15-C16
22	C	510	CLA	C6-C7-C8-C9
22	a	403	CLA	C11-C12-C13-C14
22	b	601	CLA	C14-C13-C15-C16
22	b	602	CLA	C14-C13-C15-C16
22	b	604	CLA	C11-C10-C8-C9
22	b	615	CLA	C14-C13-C15-C16
22	c	502	CLA	C11-C12-C13-C14
22	c	502	CLA	C14-C13-C15-C16
22	d	403	CLA	C11-C10-C8-C9
23	d	401	PHO	C6-C7-C8-C9
27	t	102	SQD	C24-C25-C26-C27
31	d	411	STE	C12-C13-C14-C15
26	a	414	LMG	C9-C8-O7-C10
27	A	410	SQD	C9-C10-C11-C12
26	M	101	LMG	C33-C34-C35-C36
27	A	412	SQD	C31-C32-C33-C34
29	C	516	DGD	C2B-C3B-C4B-C5B
22	B	608	CLA	C13-C15-C16-C17
22	c	505	CLA	C10-C11-C12-C13
22	C	506	CLA	C1A-C2A-CAA-CBA
22	C	508	CLA	C1A-C2A-CAA-CBA
22	c	511	CLA	C1A-C2A-CAA-CBA
31	b	626	STE	C2-C3-C4-C5
31	M	102	STE	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
31	a	413	STE	C12-C13-C14-C15
31	B	619	STE	C12-C13-C14-C15
26	M	101	LMG	C39-C40-C41-C42
22	B	614	CLA	C2B-C3B-CAB-CBB
22	H	101	CLA	C2B-C3B-CAB-CBB
30	K	102	BCR	C23-C24-C25-C30
30	k	102	BCR	C5-C6-C7-C8
30	k	102	BCR	C23-C24-C25-C26
30	t	101	BCR	C1-C6-C7-C8
30	t	101	BCR	C5-C6-C7-C8
30	x	101	BCR	C23-C24-C25-C26
28	A	411	LHG	C23-C24-C25-C26
31	X	101	STE	O1-C1-C2-C3
31	b	626	STE	O1-C1-C2-C3
31	b	626	STE	O2-C1-C2-C3
28	b	623	LHG	C24-C25-C26-C27
28	d	408	LHG	C24-C25-C26-C27
29	C	516	DGD	O6D-C5D-C6D-O5D
29	h	101	DGD	CBB-CCB-CDB-CEB
22	C	501	CLA	C4C-C3C-CAC-CBC
31	C	521	STE	C5-C6-C7-C8
26	D	408	LMG	C32-C33-C34-C35
31	X	101	STE	C13-C14-C15-C16
22	B	614	CLA	C6-C7-C8-C10
22	D	405	CLA	C12-C13-C15-C16
22	b	613	CLA	C11-C12-C13-C15
22	b	614	CLA	C6-C7-C8-C10
22	b	615	CLA	C12-C13-C15-C16
22	c	503	CLA	C11-C12-C13-C15
22	c	504	CLA	C11-C12-C13-C14
22	B	613	CLA	C2A-CAA-CBA-CGA
31	X	101	STE	O2-C1-C2-C3
31	d	411	STE	O2-C1-C2-C3
34	f	101	HEC	CAD-CBD-CGD-O2D
28	L	102	LHG	C10-C11-C12-C13
26	m	101	LMG	C14-C15-C16-C17
28	D	410	LHG	C9-C10-C11-C12
30	t	101	BCR	C11-C12-C13-C35
29	h	101	DGD	C9B-CAB-CBB-CCB
22	c	508	CLA	C4-C3-C5-C6
22	b	603	CLA	C8-C10-C11-C12
22	B	607	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	D	407	PL9	C33-C34-C36-C37
22	D	403	CLA	C2-C1-O2A-CGA
29	H	103	DGD	C9B-CAB-CBB-CCB
31	C	519	STE	O2-C1-C2-C3
22	c	513	CLA	C13-C15-C16-C17
26	c	520	LMG	C29-C30-C31-C32
34	f	101	HEC	CAD-CBD-CGD-O1D
22	B	605	CLA	C14-C13-C15-C16
22	C	510	CLA	C14-C13-C15-C16
22	D	404	CLA	C8-C10-C11-C12
29	C	518	DGD	C8B-C9B-CAB-CBB
29	C	518	DGD	CDA-CEA-CFA-CGA
27	A	410	SQD	C31-C32-C33-C34
28	A	411	LHG	C33-C34-C35-C36
26	D	408	LMG	C22-C23-C24-C25
30	B	618	BCR	C6-C7-C8-C9
30	B	618	BCR	C22-C23-C24-C25
31	x	102	STE	C10-C11-C12-C13
22	A	405	CLA	C4-C3-C5-C6
22	d	403	CLA	C4-C3-C5-C6
31	M	102	STE	O2-C1-C2-C3
22	b	615	CLA	C2-C3-C5-C6
25	a	409	PL9	C18-C19-C21-C22
25	a	409	PL9	C29-C31-C32-C33
22	c	505	CLA	O1A-CGA-O2A-C1
25	A	408	PL9	C47-C48-C49-C51
26	b	622	LMG	C14-C15-C16-C17
26	c	520	LMG	C39-C40-C41-C42
28	D	413	LHG	O6-C4-C5-O7
27	A	412	SQD	C35-C36-C37-C38
26	M	101	LMG	C18-C19-C20-C21
31	B	622	STE	O2-C1-C2-C3
22	C	506	CLA	C3-C5-C6-C7
28	b	623	LHG	C26-C27-C28-C29
31	M	104	STE	C11-C12-C13-C14
31	c	519	STE	C14-C15-C16-C17
29	C	516	DGD	C8A-C9A-CAA-CBA
31	J	101	STE	C7-C8-C9-C10
26	M	101	LMG	O6-C5-C6-O5
27	B	621	SQD	C34-C35-C36-C37
27	A	410	SQD	O49-C7-O47-C45
30	x	101	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
22	d	403	CLA	C2C-C3C-CAC-CBC
29	c	517	DGD	C5A-C6A-C7A-C8A
22	A	402	CLA	C4C-C3C-CAC-CBC
29	c	515	DGD	C6A-C7A-C8A-C9A
29	C	518	DGD	CDB-CEB-CFB-CGB
27	D	409	SQD	C45-C46-O48-C23
22	B	608	CLA	C4-C3-C5-C6
31	j	101	STE	C5-C6-C7-C8
26	b	622	LMG	O1-C7-C8-O7
31	b	621	STE	O1-C1-C2-C3
22	b	602	CLA	C12-C13-C15-C16
30	C	515	BCR	C15-C16-C17-C18
31	C	519	STE	O1-C1-C2-C3
30	H	102	BCR	C21-C22-C23-C24
22	B	612	CLA	C14-C13-C15-C16
22	b	602	CLA	C11-C10-C8-C9
27	L	101	SQD	C45-C44-O6-C1
27	L	101	SQD	C5-C6-S-O8
28	D	413	LHG	C29-C30-C31-C32
31	b	625	STE	C11-C12-C13-C14
22	B	603	CLA	C2-C1-O2A-CGA
22	B	615	CLA	C2-C1-O2A-CGA
22	c	513	CLA	C8-C10-C11-C12
29	h	101	DGD	O2G-C1B-C2B-C3B
22	C	511	CLA	C3-C5-C6-C7
26	b	622	LMG	C40-C41-C42-C43
26	A	409	LMG	C7-C8-O7-C10
26	c	518	LMG	C36-C37-C38-C39
31	B	624	STE	C13-C14-C15-C16
31	t	103	STE	O2-C1-C2-C3
22	b	616	CLA	C11-C12-C13-C15
34	v	201	HEC	CAD-CBD-CGD-O2D
29	C	516	DGD	C4E-C5E-C6E-O5E
26	B	620	LMG	O10-C28-C29-C30
28	A	411	LHG	C29-C30-C31-C32
31	B	622	STE	C5-C6-C7-C8
22	c	505	CLA	CBA-CGA-O2A-C1
31	t	103	STE	O1-C1-C2-C3
26	A	409	LMG	C7-C8-C9-O8
29	h	101	DGD	C1G-C2G-C3G-O3G
28	D	410	LHG	C33-C34-C35-C36
34	V	201	HEC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	c	502	CLA	C13-C15-C16-C17
30	b	619	BCR	C9-C10-C11-C12
30	c	514	BCR	C15-C16-C17-C18
22	c	502	CLA	O1A-CGA-O2A-C1
22	b	605	CLA	C10-C11-C12-C13
28	L	102	LHG	C11-C10-C9-C8
26	A	409	LMG	C39-C40-C41-C42
31	C	519	STE	C6-C7-C8-C9
34	V	201	HEC	CAD-CBD-CGD-O2D
22	C	505	CLA	C14-C13-C15-C16
22	C	506	CLA	C11-C12-C13-C14
22	b	606	CLA	C11-C12-C13-C14
22	b	608	CLA	C11-C12-C13-C14
22	b	612	CLA	C14-C13-C15-C16
31	H	104	STE	C14-C15-C16-C17
31	b	626	STE	C11-C10-C9-C8
29	c	516	DGD	C9B-CAB-CBB-CCB
22	b	601	CLA	CAA-CBA-CGA-O2A
28	b	623	LHG	O6-C4-C5-C6
30	H	102	BCR	C17-C18-C19-C20
26	B	620	LMG	C17-C18-C19-C20
25	d	407	PL9	C37-C38-C39-C40
22	B	607	CLA	C13-C15-C16-C17
22	B	609	CLA	C2A-CAA-CBA-CGA
22	c	507	CLA	C2A-CAA-CBA-CGA
22	A	403	CLA	C12-C13-C15-C16
22	B	602	CLA	C11-C10-C8-C7
22	B	608	CLA	C11-C12-C13-C15
22	c	502	CLA	C11-C12-C13-C15
22	c	511	CLA	C6-C7-C8-C10
23	a	404	PHO	C6-C7-C8-C10
22	b	602	CLA	C2B-C3B-CAB-CBB
22	b	610	CLA	C2B-C3B-CAB-CBB
30	k	103	BCR	C23-C24-C25-C26
29	A	413	DGD	C3B-C4B-C5B-C6B
34	v	201	HEC	C2B-C3B-CAB-CBB
28	d	408	LHG	O9-C7-O7-C5
31	d	411	STE	C6-C7-C8-C9
22	C	506	CLA	C2-C1-O2A-CGA
22	c	502	CLA	C2-C1-O2A-CGA
34	v	201	HEC	CAD-CBD-CGD-O1D
26	d	410	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	B	623	STE	C13-C14-C15-C16
29	C	517	DGD	O2G-C1B-C2B-C3B
22	B	608	CLA	C2-C3-C5-C6
22	C	503	CLA	C10-C11-C12-C13
29	C	516	DGD	C9B-CAB-CBB-CCB
29	c	515	DGD	C9A-CAA-CBA-CCA
22	B	601	CLA	C15-C16-C17-C18
22	B	601	CLA	C10-C11-C12-C13
22	c	502	CLA	CBA-CGA-O2A-C1
29	c	516	DGD	O2G-C1B-C2B-C3B
26	B	620	LMG	C16-C17-C18-C19
27	D	409	SQD	C32-C33-C34-C35
22	c	509	CLA	CAA-CBA-CGA-O1A
28	D	413	LHG	O10-C23-C24-C25
22	C	507	CLA	CBD-CGD-O2D-CED
29	C	518	DGD	CAB-CBB-CCB-CDB
31	L	103	STE	C4-C5-C6-C7
30	K	101	BCR	C18-C19-C20-C21
28	a	411	LHG	O8-C23-C24-C25
22	A	405	CLA	C2-C3-C5-C6
25	a	409	PL9	C23-C24-C26-C27
31	a	413	STE	C9-C10-C11-C12
34	F	101	HEC	CAD-CBD-CGD-O1D
22	c	503	CLA	C8-C10-C11-C12
26	M	101	LMG	C20-C21-C22-C23
27	B	621	SQD	C27-C28-C29-C30
31	b	624	STE	O1-C1-C2-C3
31	x	102	STE	O2-C1-C2-C3
34	F	101	HEC	CAD-CBD-CGD-O2D
31	H	104	STE	C15-C16-C17-C18
22	c	503	CLA	C11-C10-C8-C9
22	B	605	CLA	C10-C11-C12-C13
29	c	515	DGD	C1G-C2G-C3G-O3G
27	D	409	SQD	C44-C45-C46-O48
22	D	405	CLA	C4B-C3B-CAB-CBB
22	b	602	CLA	C1A-C2A-CAA-CBA
22	b	604	CLA	C1A-C2A-CAA-CBA
22	d	403	CLA	C4B-C3B-CAB-CBB
31	b	621	STE	O2-C1-C2-C3
31	b	624	STE	O2-C1-C2-C3
31	x	102	STE	O1-C1-C2-C3
31	C	521	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
29	c	516	DGD	O6D-C1D-O3G-C3G
26	m	101	LMG	O8-C28-C29-C30
28	A	411	LHG	C30-C31-C32-C33
22	c	508	CLA	C2-C3-C5-C6
31	X	101	STE	C15-C16-C17-C18
30	K	101	BCR	C7-C8-C9-C10
30	b	617	BCR	C11-C12-C13-C14
30	d	406	BCR	C21-C22-C23-C24
30	k	102	BCR	C11-C12-C13-C14
22	b	604	CLA	C8-C10-C11-C12
28	d	409	LHG	C9-C10-C11-C12
22	b	601	CLA	O1A-CGA-O2A-C1
22	C	501	CLA	C16-C17-C18-C20
22	c	512	CLA	C5-C6-C7-C8
31	M	104	STE	C7-C8-C9-C10
31	M	103	STE	C1-C2-C3-C4
22	C	506	CLA	C13-C15-C16-C17
22	B	612	CLA	C6-C7-C8-C10
22	B	613	CLA	C11-C10-C8-C7
22	C	505	CLA	C6-C7-C8-C10
22	C	508	CLA	C12-C13-C15-C16
22	H	101	CLA	C6-C7-C8-C10
22	a	405	CLA	C12-C13-C15-C16
22	b	607	CLA	C11-C10-C8-C7
22	b	612	CLA	C11-C10-C8-C7
22	c	505	CLA	C12-C13-C15-C16
22	c	508	CLA	C11-C12-C13-C15
22	c	512	CLA	C11-C10-C8-C7
22	B	612	CLA	CAA-CBA-CGA-O2A
28	L	102	LHG	O7-C7-C8-C9
31	I	102	STE	C7-C8-C9-C10
31	b	626	STE	C15-C16-C17-C18
31	B	625	STE	C2-C3-C4-C5
28	d	409	LHG	C32-C33-C34-C35
29	c	517	DGD	O1G-C1A-C2A-C3A
22	c	507	CLA	O1A-CGA-O2A-C1
26	Y	101	LMG	C30-C31-C32-C33
22	c	507	CLA	CBA-CGA-O2A-C1
28	D	411	LHG	C2-C3-O3-P
22	H	101	CLA	C3A-C2A-CAA-CBA
22	b	601	CLA	C2C-C3C-CAC-CBC
22	b	603	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
30	T	101	BCR	C16-C17-C18-C19
30	k	102	BCR	C12-C13-C14-C15
26	B	620	LMG	O7-C10-C11-C12
22	B	602	CLA	C2A-CAA-CBA-CGA
22	b	614	CLA	C2A-CAA-CBA-CGA
22	C	505	CLA	C6-C7-C8-C9
22	b	612	CLA	C11-C10-C8-C9
22	c	505	CLA	C6-C7-C8-C9
22	c	508	CLA	C11-C12-C13-C14
22	c	505	CLA	CBD-CGD-O2D-CED
31	b	624	STE	C5-C6-C7-C8
26	d	410	LMG	O9-C10-C11-C12
28	b	623	LHG	O10-C23-O8-C6
26	Y	101	LMG	O9-C10-C11-C12
29	c	515	DGD	O1B-C1B-C2B-C3B
28	d	408	LHG	C13-C14-C15-C16
31	B	623	STE	C9-C10-C11-C12
30	C	514	BCR	C11-C12-C13-C14
22	B	612	CLA	CAA-CBA-CGA-O1A
27	a	410	SQD	O49-C7-C8-C9
26	m	101	LMG	C8-C7-O1-C1
26	A	409	LMG	O7-C8-C9-O8
22	b	601	CLA	CAA-CBA-CGA-O1A
28	b	623	LHG	O8-C23-C24-C25
31	C	520	STE	C15-C16-C17-C18
26	c	521	LMG	C16-C17-C18-C19
26	b	622	LMG	O10-C28-C29-C30
27	A	410	SQD	O49-C7-C8-C9
28	d	409	LHG	O10-C23-C24-C25
25	A	408	PL9	C21-C22-C23-C24
27	L	101	SQD	C10-C11-C12-C13
28	a	411	LHG	O10-C23-C24-C25
22	C	504	CLA	CAD-CBD-CGD-O2D
26	b	622	LMG	O8-C28-C29-C30
22	C	509	CLA	C5-C6-C7-C8
28	b	623	LHG	C25-C26-C27-C28
22	d	403	CLA	C2-C1-O2A-CGA
22	c	510	CLA	CAA-CBA-CGA-O2A
27	A	410	SQD	O47-C7-C8-C9
26	c	520	LMG	C38-C39-C40-C41
31	d	411	STE	C11-C10-C9-C8
22	C	509	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	L	101	SQD	C11-C10-C9-C8
28	D	411	LHG	O10-C23-C24-C25
22	b	613	CLA	CAA-CBA-CGA-O2A
28	D	413	LHG	O8-C23-C24-C25
26	A	409	LMG	C40-C41-C42-C43
27	L	101	SQD	C15-C16-C17-C18
29	c	515	DGD	O2G-C1B-C2B-C3B
31	R	101	STE	O1-C1-C2-C3
22	B	615	CLA	C4C-C3C-CAC-CBC

There are no ring outliers.

102 monomers are involved in 177 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	606	CLA	3	0
31	I	102	STE	1	0
29	C	517	DGD	2	0
30	B	618	BCR	2	0
30	T	101	BCR	4	0
22	b	607	CLA	3	0
30	K	102	BCR	1	0
28	d	408	LHG	3	0
31	b	621	STE	2	0
22	B	608	CLA	3	0
26	D	408	LMG	1	0
22	a	402	CLA	3	0
26	m	101	LMG	1	0
23	d	401	PHO	1	0
30	b	618	BCR	1	0
22	B	615	CLA	1	0
22	D	403	CLA	6	0
34	F	101	HEC	5	0
22	B	603	CLA	4	0
22	B	606	CLA	1	0
22	b	614	CLA	2	0
30	d	406	BCR	5	0
22	C	511	CLA	1	0
22	b	602	CLA	1	0
22	B	607	CLA	2	0
25	d	407	PL9	1	0
22	c	511	CLA	2	0
27	f	102	SQD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	B	617	BCR	6	0
25	a	409	PL9	1	0
31	X	101	STE	4	0
25	A	408	PL9	4	0
22	b	601	CLA	3	0
31	J	101	STE	1	0
30	b	617	BCR	1	0
30	k	102	BCR	1	0
31	b	629	STE	1	0
22	c	502	CLA	1	0
22	B	609	CLA	1	0
22	c	503	CLA	2	0
30	k	103	BCR	1	0
28	D	413	LHG	1	0
22	c	507	CLA	3	0
28	b	623	LHG	5	0
30	D	406	BCR	3	0
31	B	623	STE	1	0
31	c	519	STE	1	0
30	k	101	BCR	1	0
22	B	604	CLA	3	0
22	B	610	CLA	1	0
22	c	504	CLA	1	0
22	b	613	CLA	3	0
30	t	101	BCR	2	0
28	D	411	LHG	3	0
30	b	619	BCR	1	0
22	b	612	CLA	1	0
34	V	201	HEC	1	0
23	a	404	PHO	1	0
22	C	504	CLA	1	0
34	f	101	HEC	5	0
28	d	409	LHG	1	0
26	M	101	LMG	1	0
22	c	501	CLA	2	0
23	D	401	PHO	3	0
27	L	101	SQD	3	0
30	a	406	BCR	2	0
22	A	402	CLA	2	0
22	C	510	CLA	1	0
31	C	520	STE	1	0
22	A	403	CLA	4	0

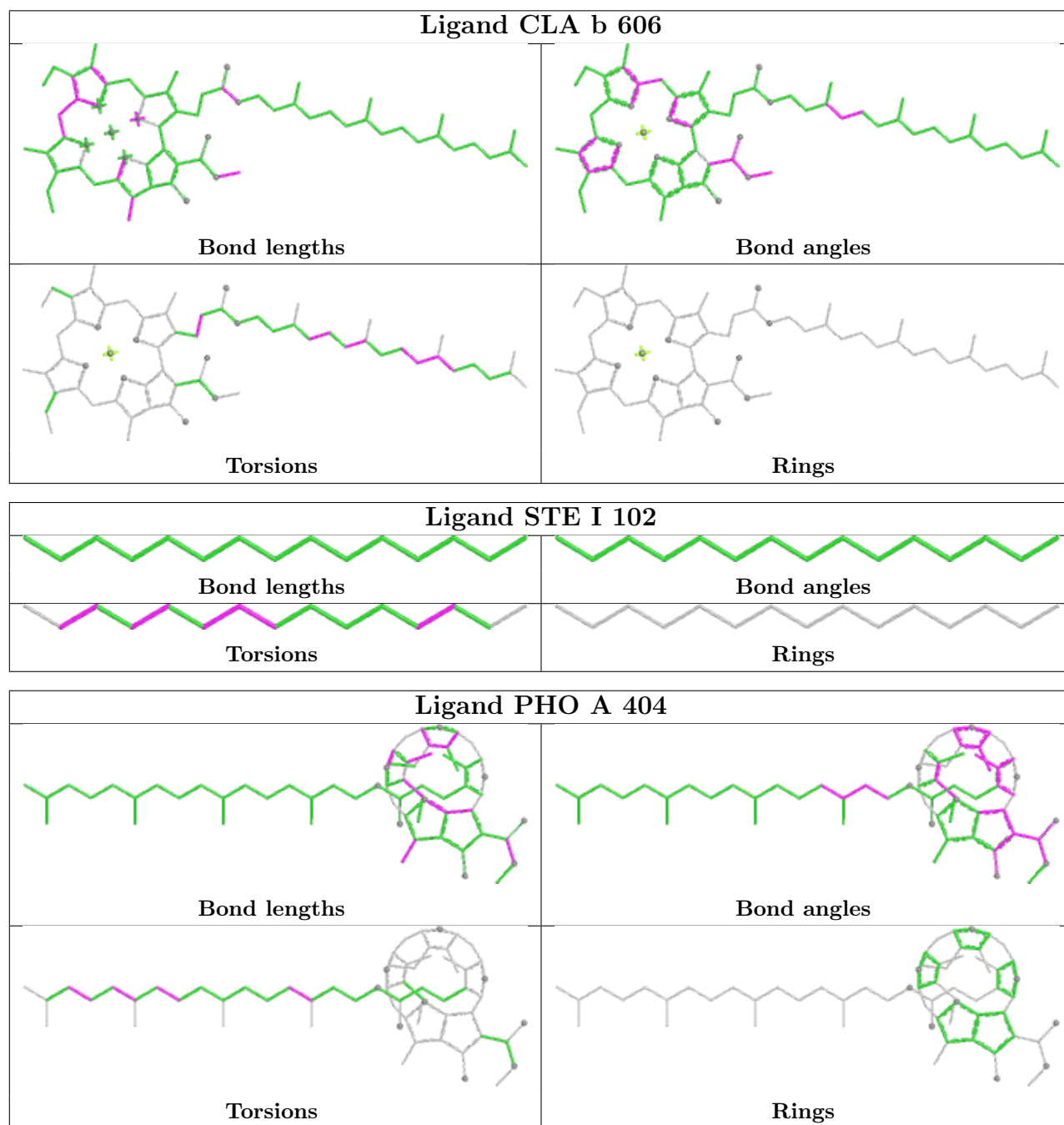
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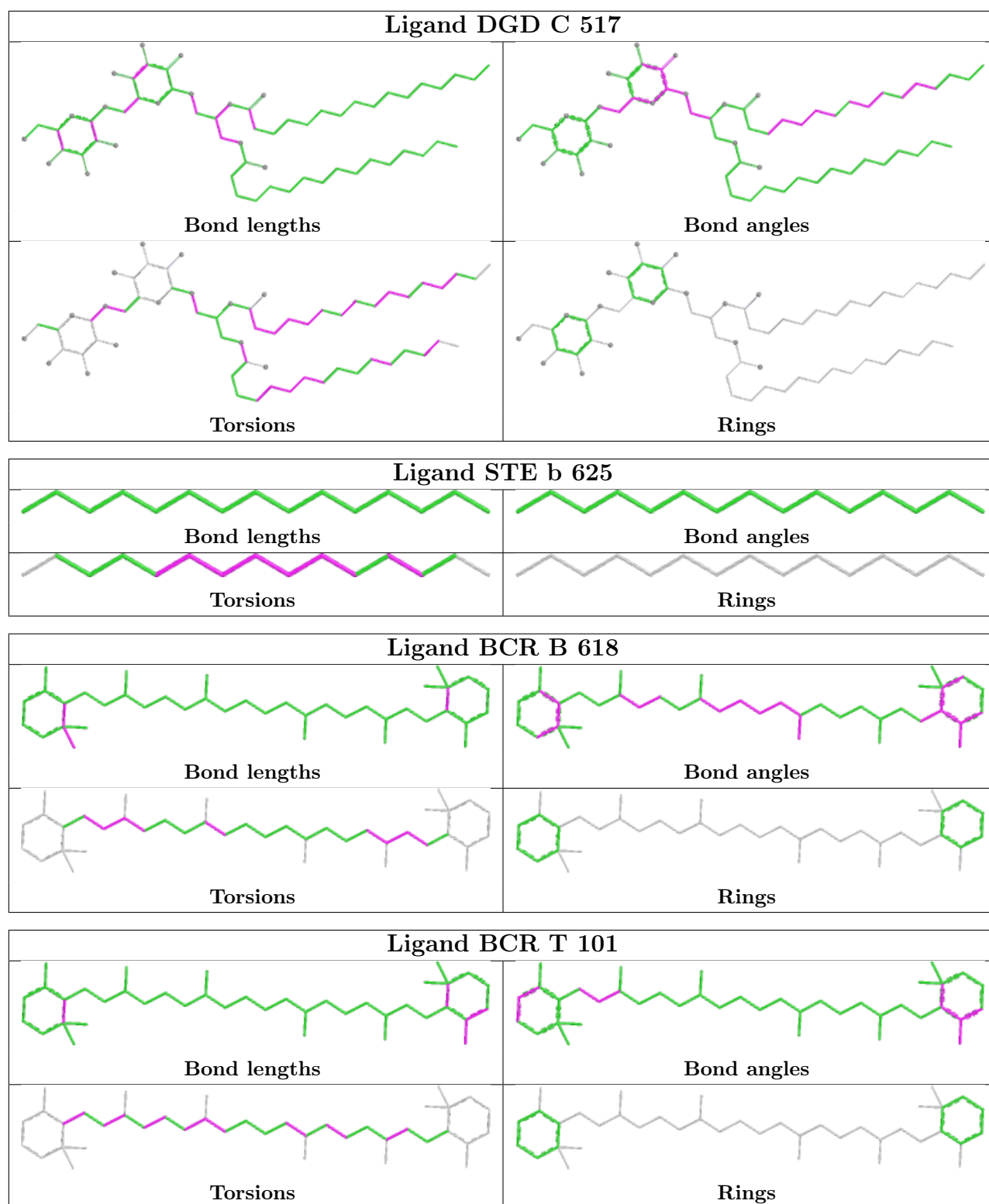
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	601	CLA	2	0
31	j	101	STE	1	0
34	v	201	HEC	4	0
31	b	628	STE	2	0
22	b	615	CLA	2	0
22	C	508	CLA	4	0
22	b	605	CLA	8	0
22	C	513	CLA	4	0
22	c	509	CLA	2	0
22	b	609	CLA	1	0
22	C	512	CLA	2	0
30	c	514	BCR	1	0
22	B	605	CLA	2	0
22	c	508	CLA	2	0
30	x	101	BCR	3	0
22	H	101	CLA	1	0
28	l	101	LHG	1	0
22	C	501	CLA	3	0
22	B	612	CLA	1	0
22	b	603	CLA	1	0
27	A	410	SQD	3	0
22	c	513	CLA	1	0
30	C	514	BCR	6	0
29	A	413	DGD	1	0
22	d	404	CLA	2	0
22	C	507	CLA	1	0
22	B	613	CLA	3	0
22	c	510	CLA	1	0
31	t	103	STE	1	0
27	A	412	SQD	1	0
22	b	610	CLA	1	0
25	D	407	PL9	2	0

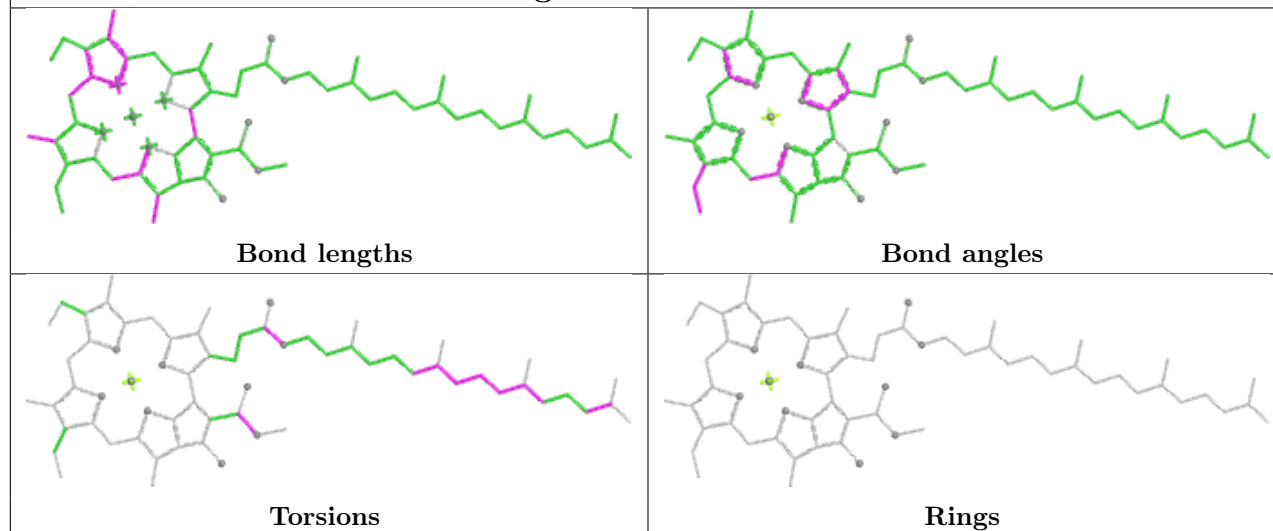
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

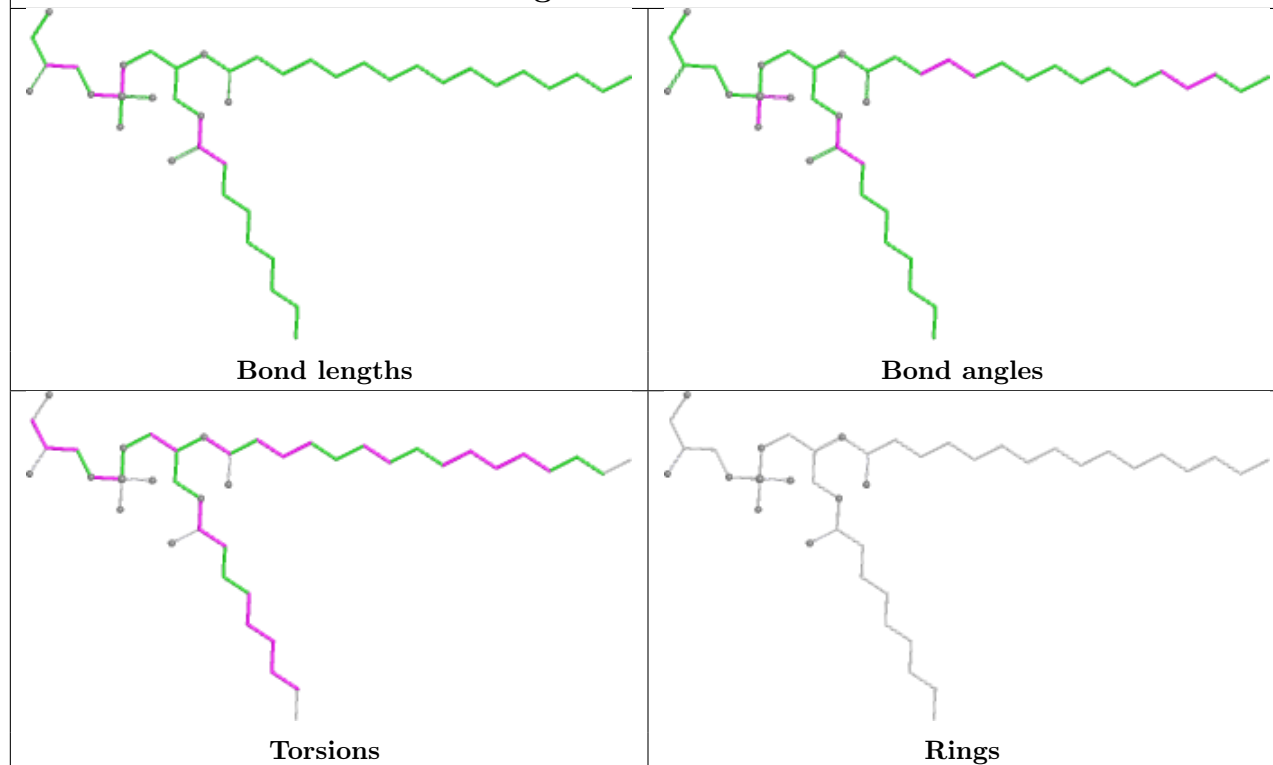




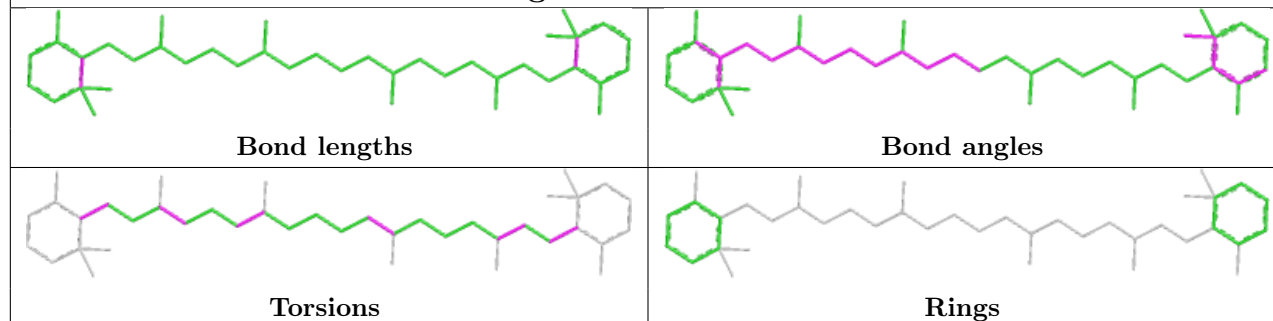
Ligand CLA b 607

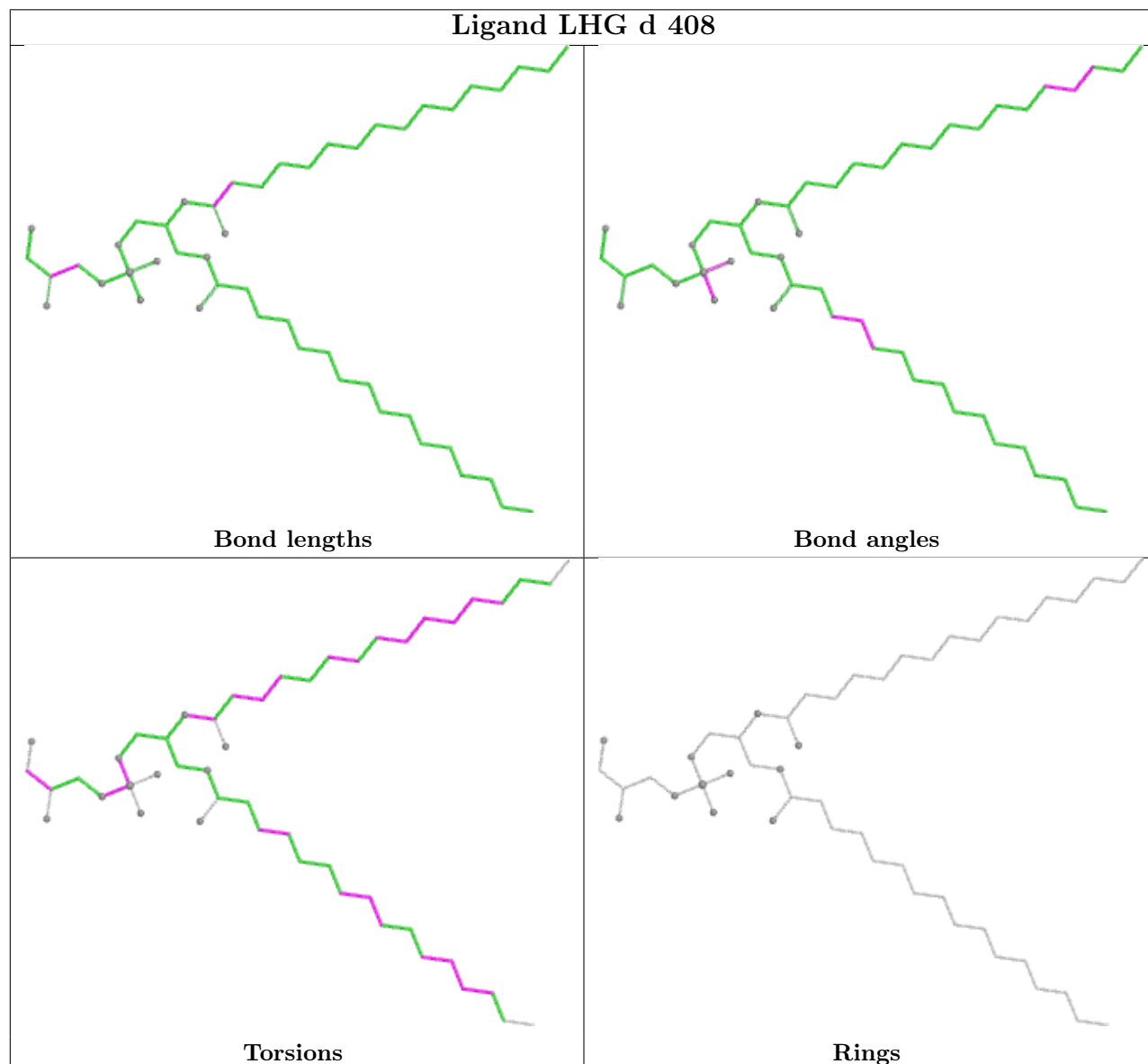
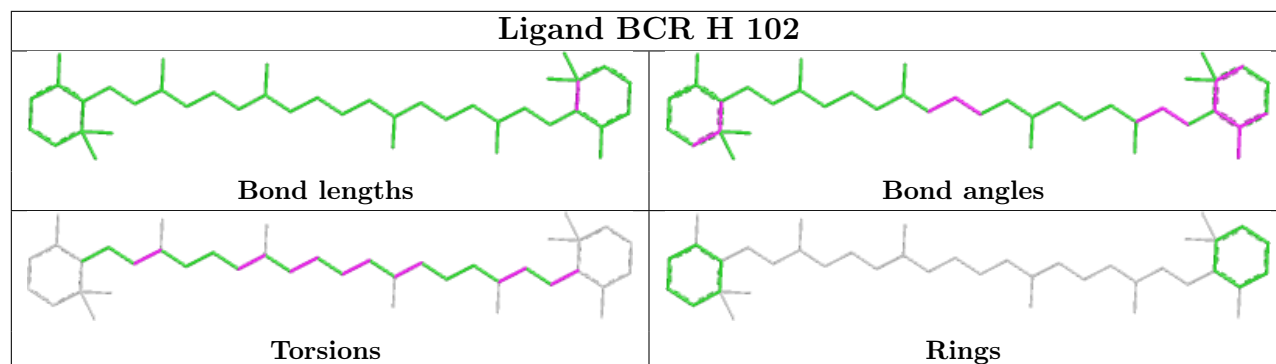


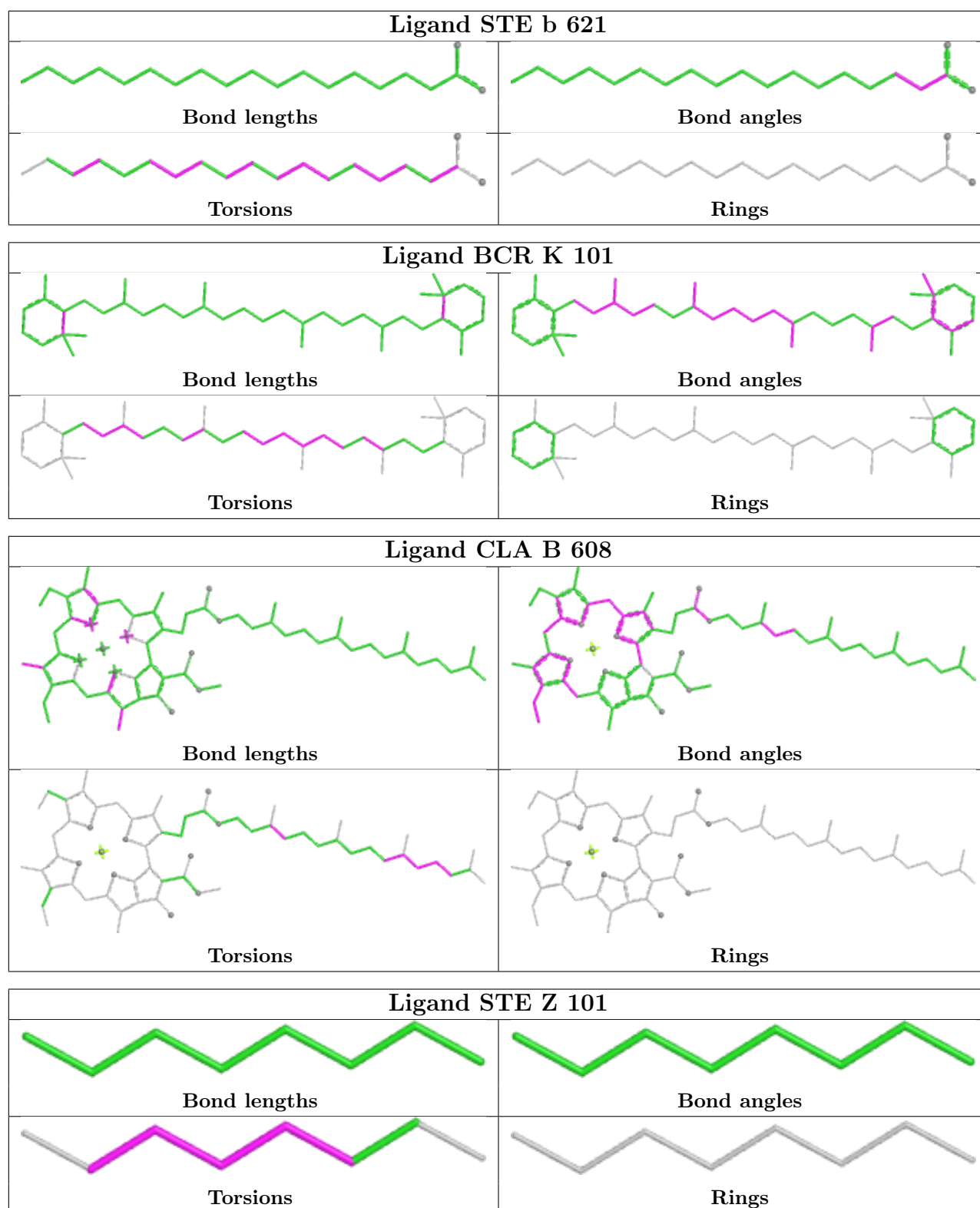
Ligand LHG a 411

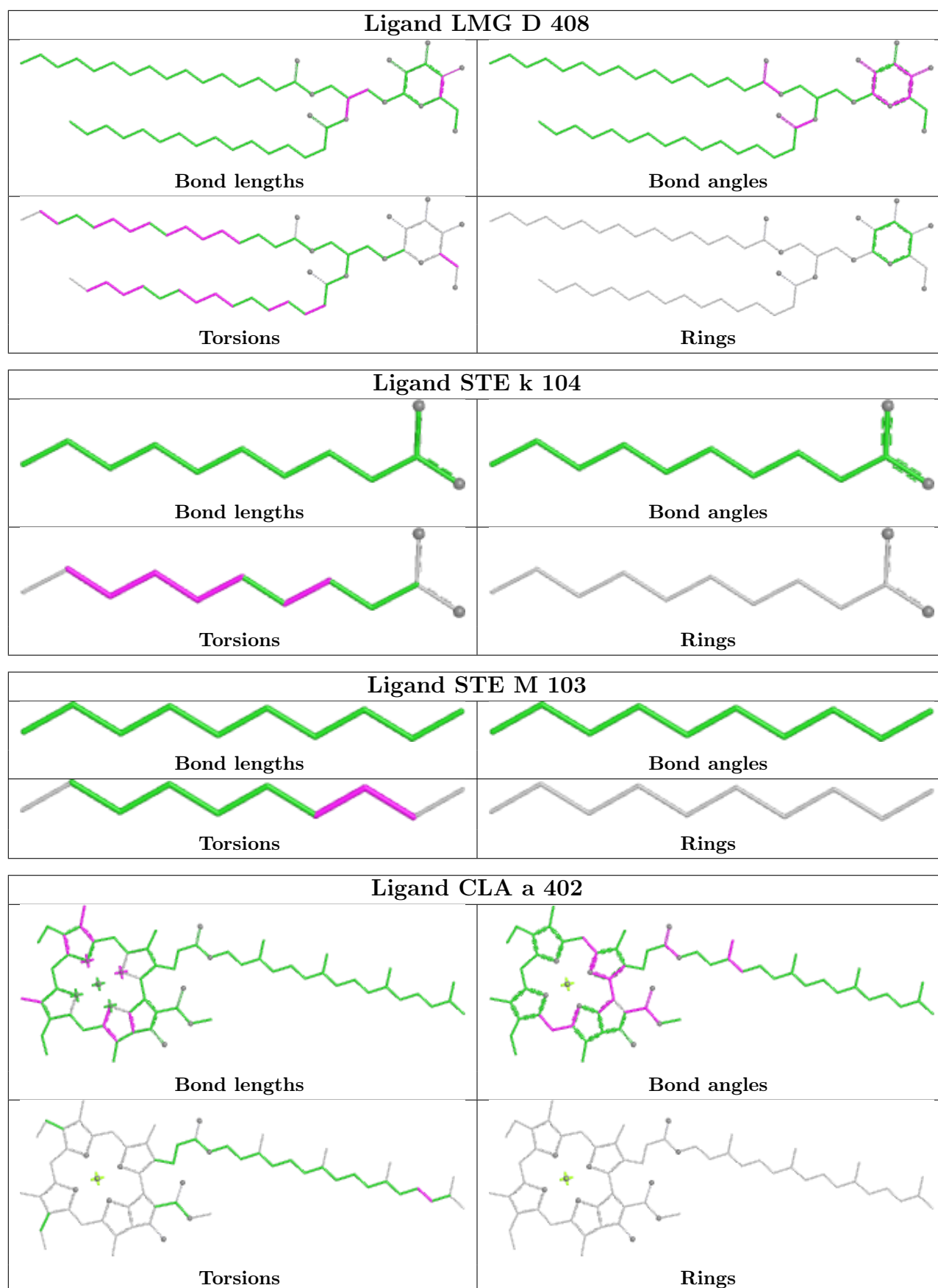


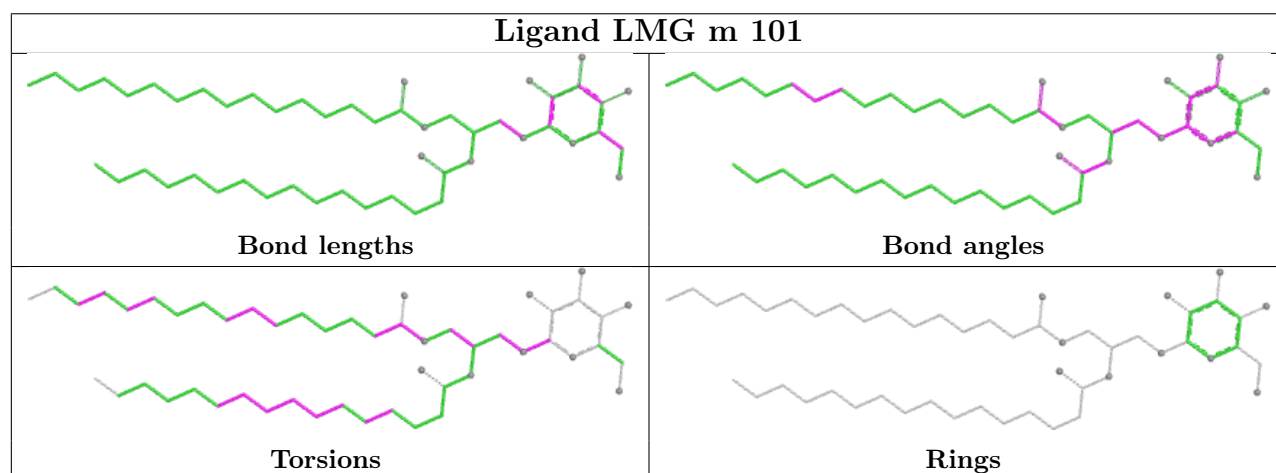
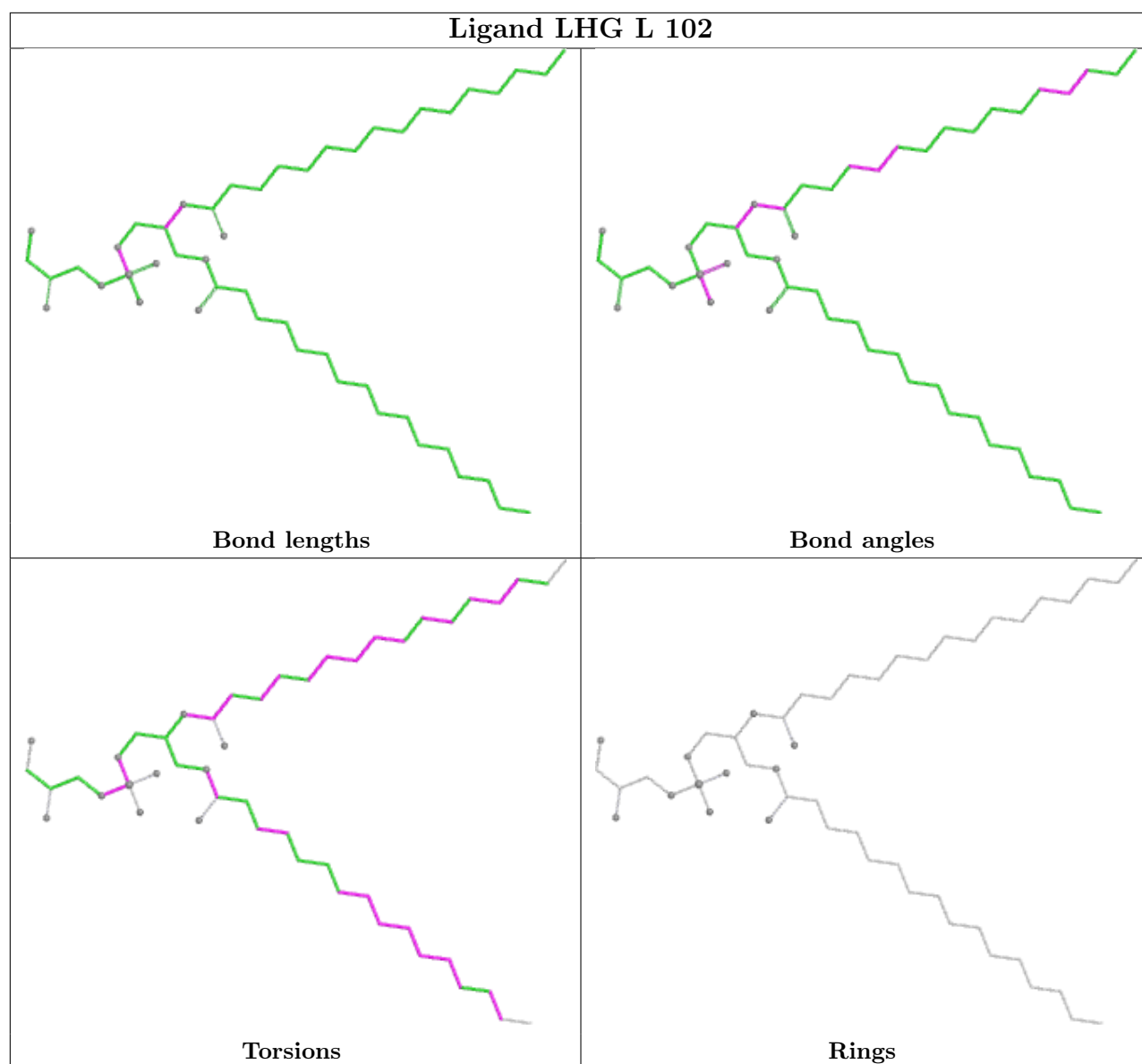
Ligand BCR K 102



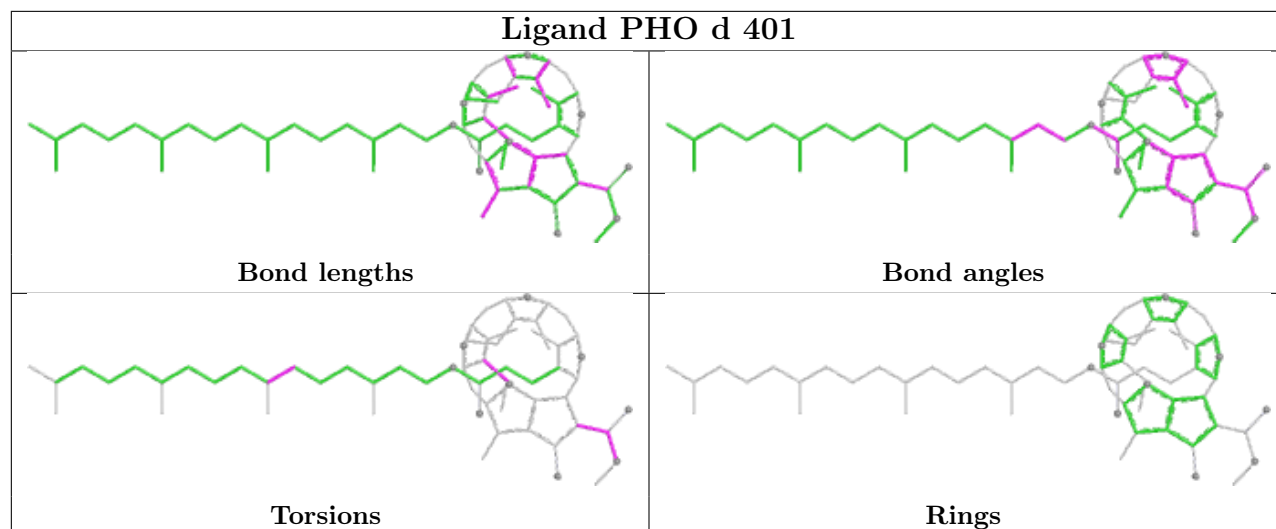




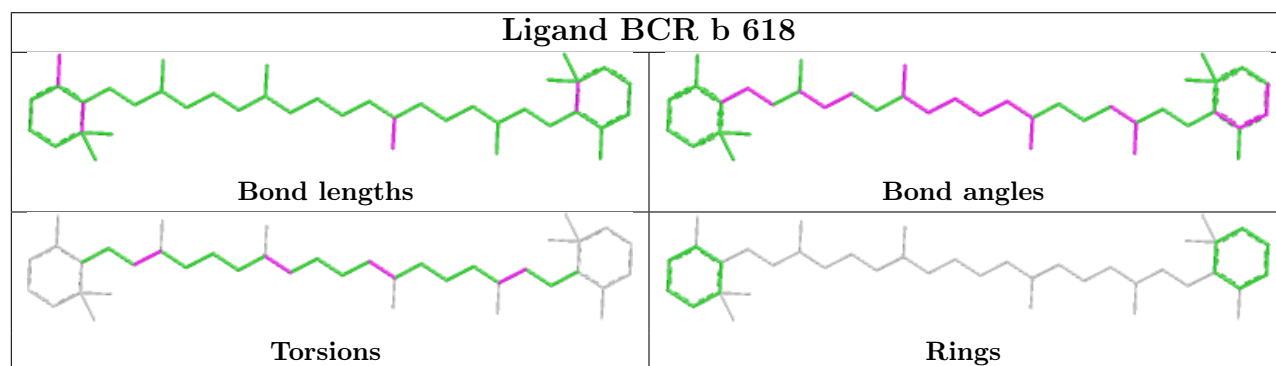




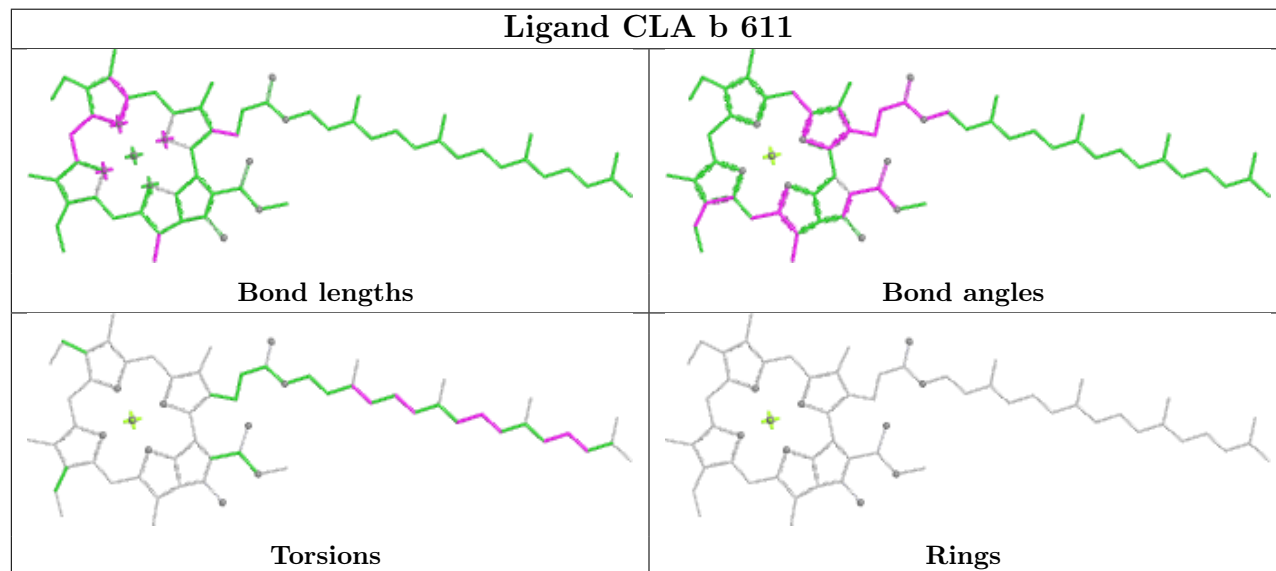
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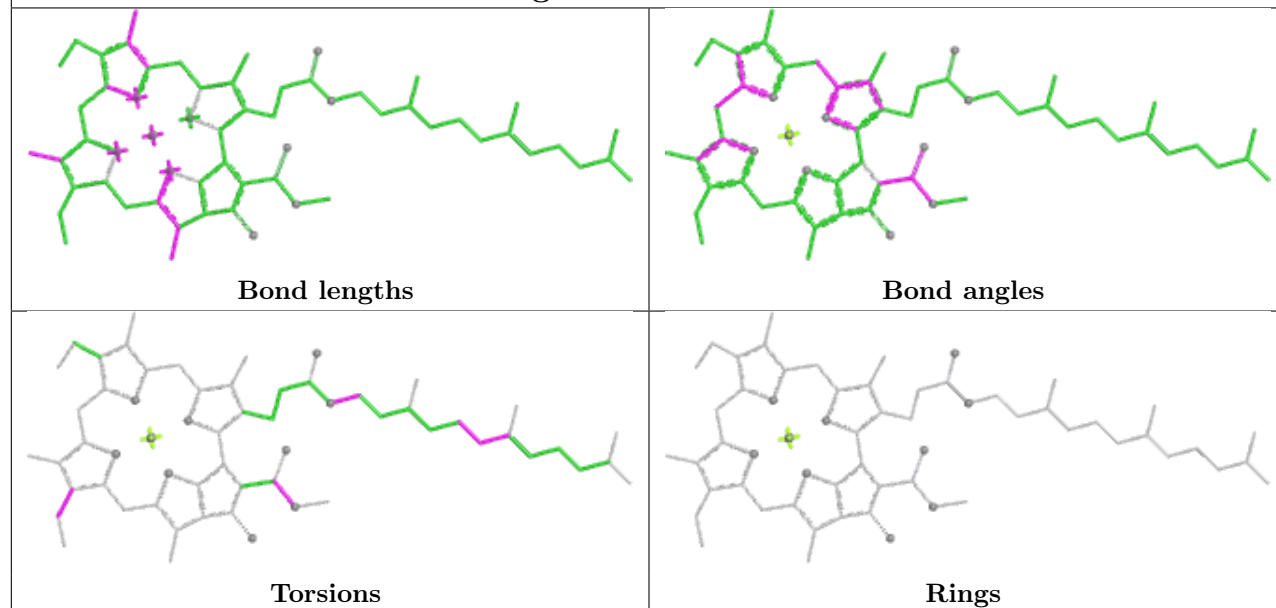
Ligand BCR b 618



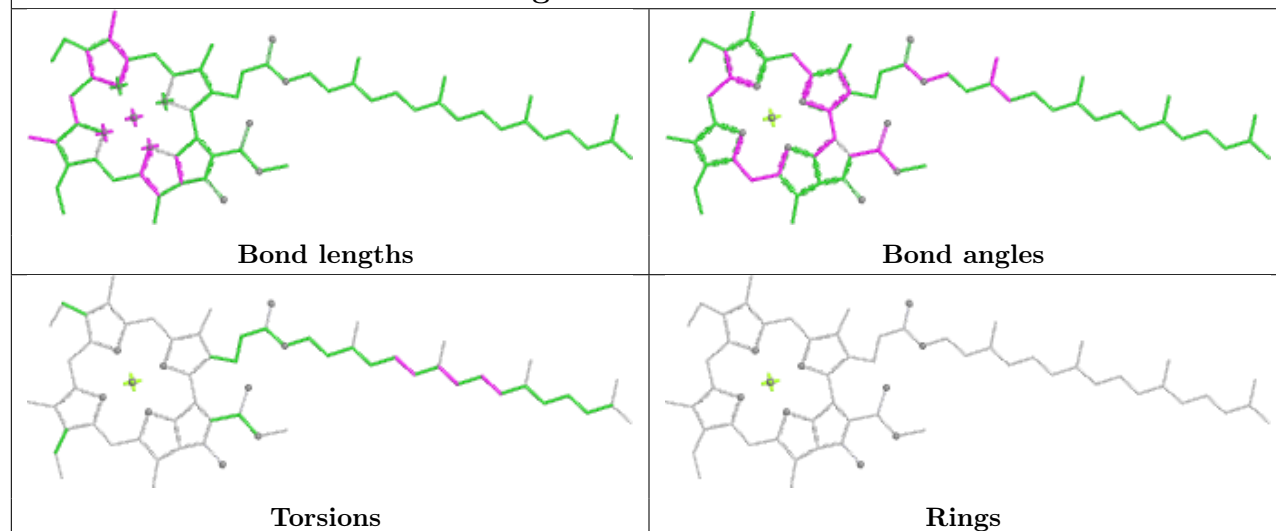
Ligand CLA b 611



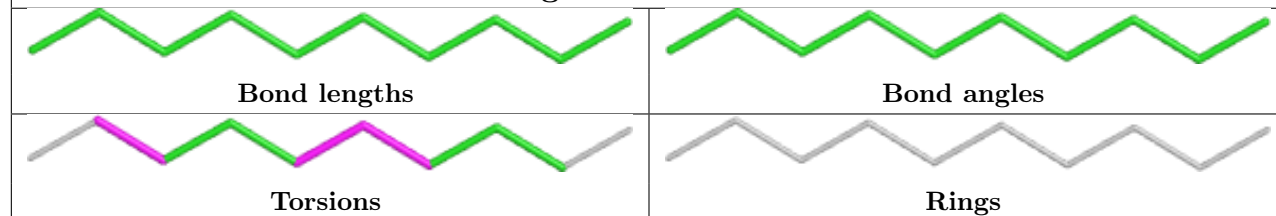
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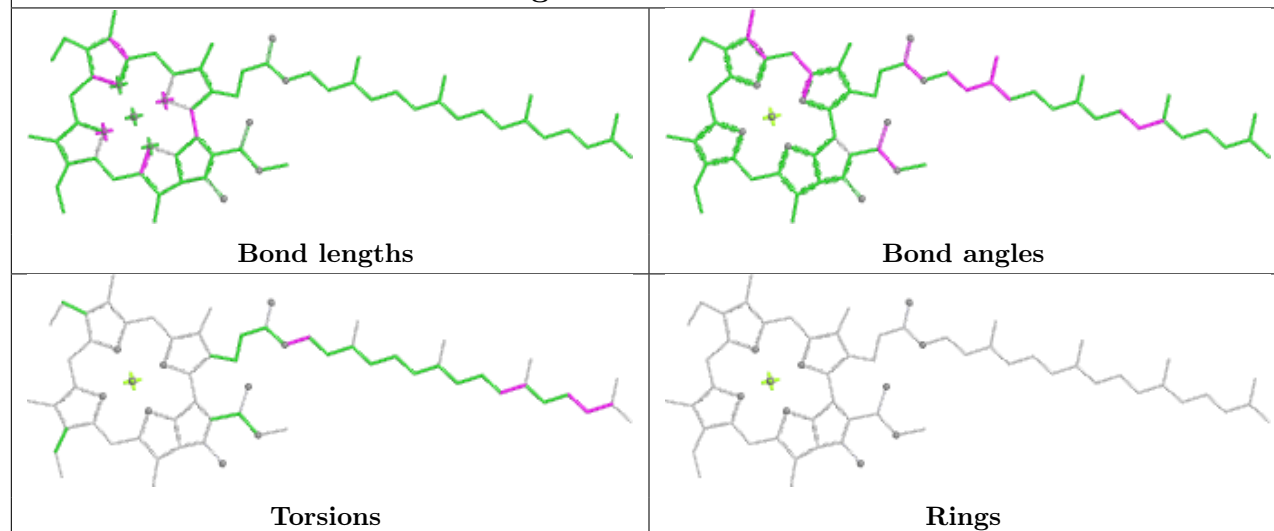
Ligand CLA C 503



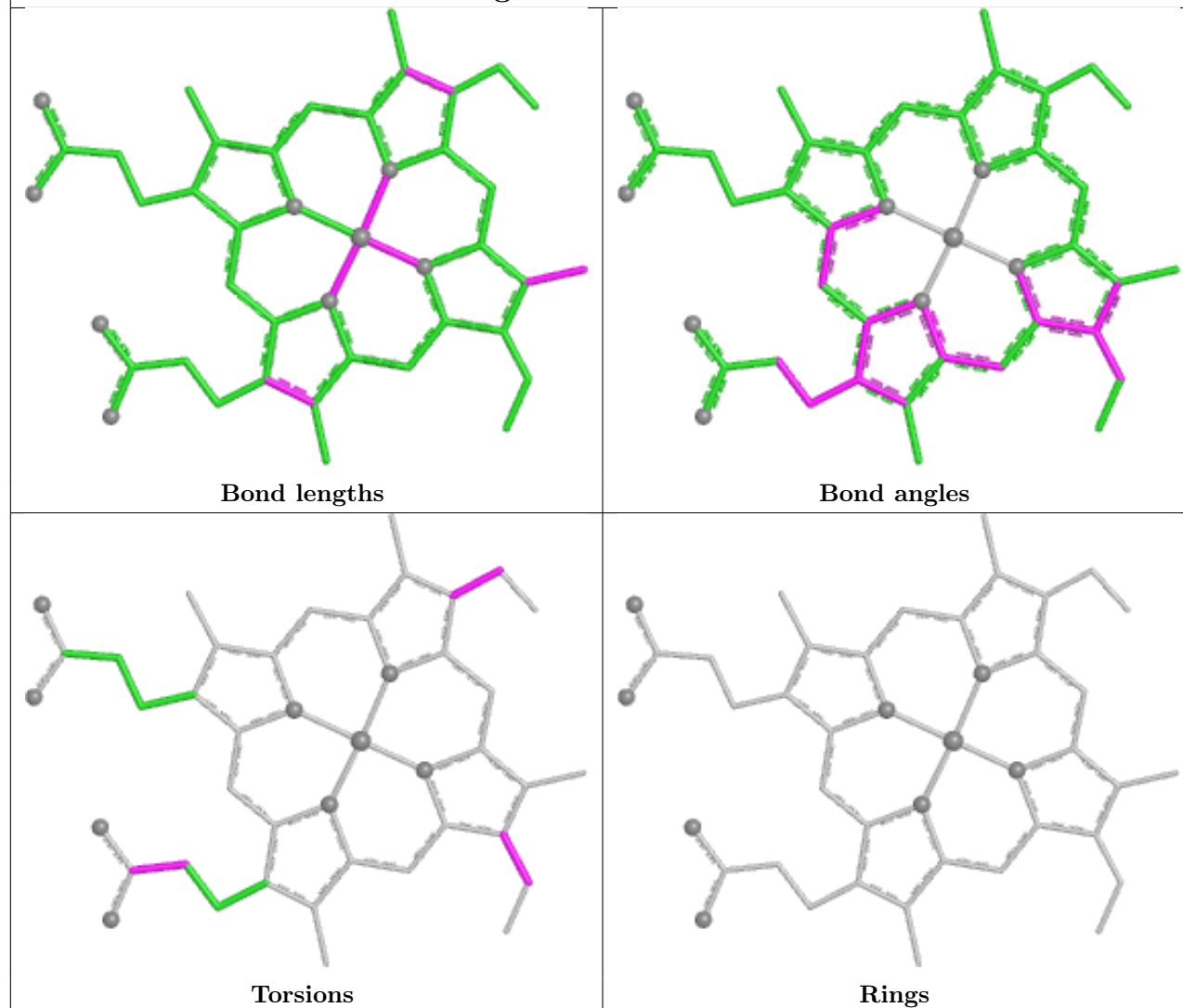
Ligand STE t 104

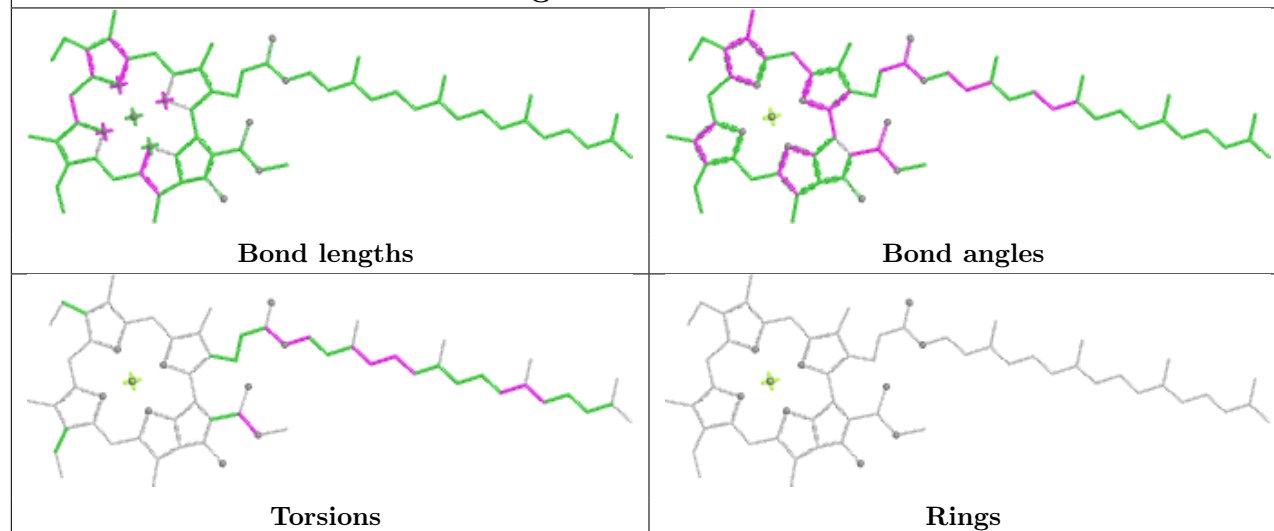
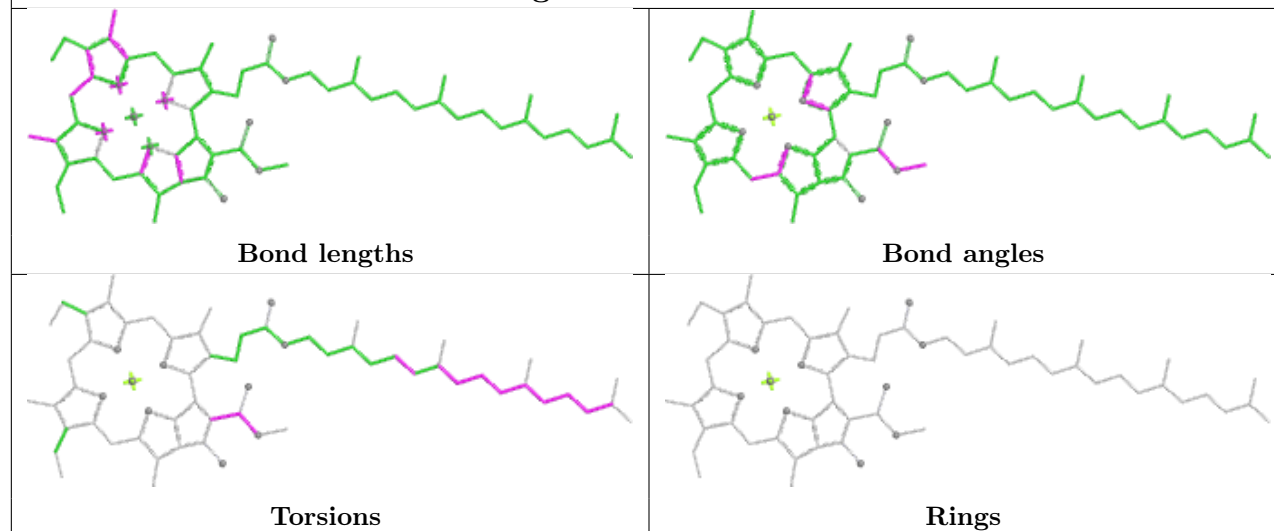
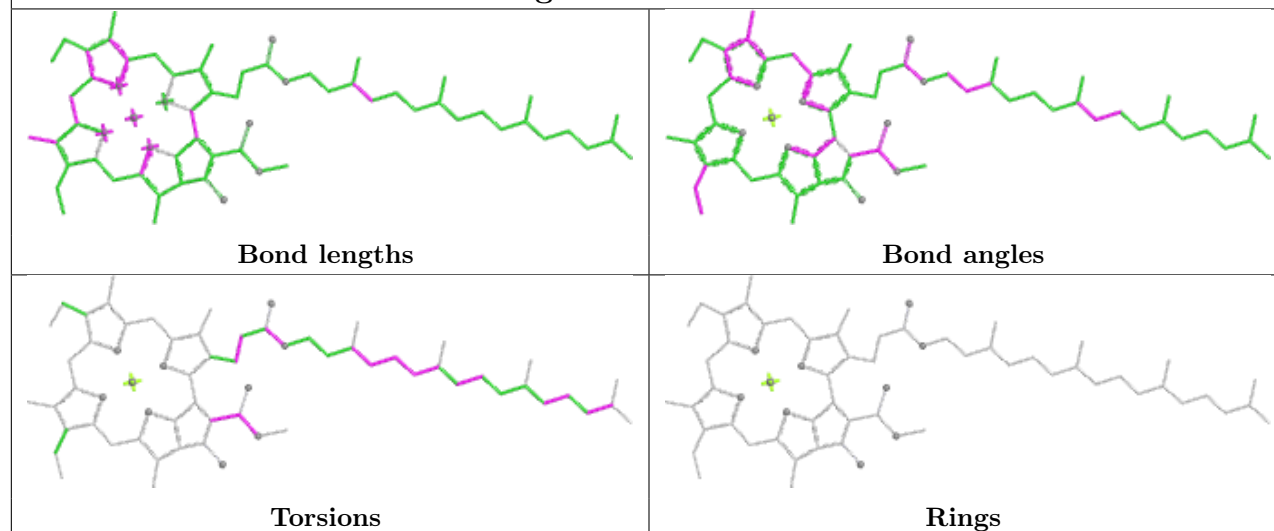


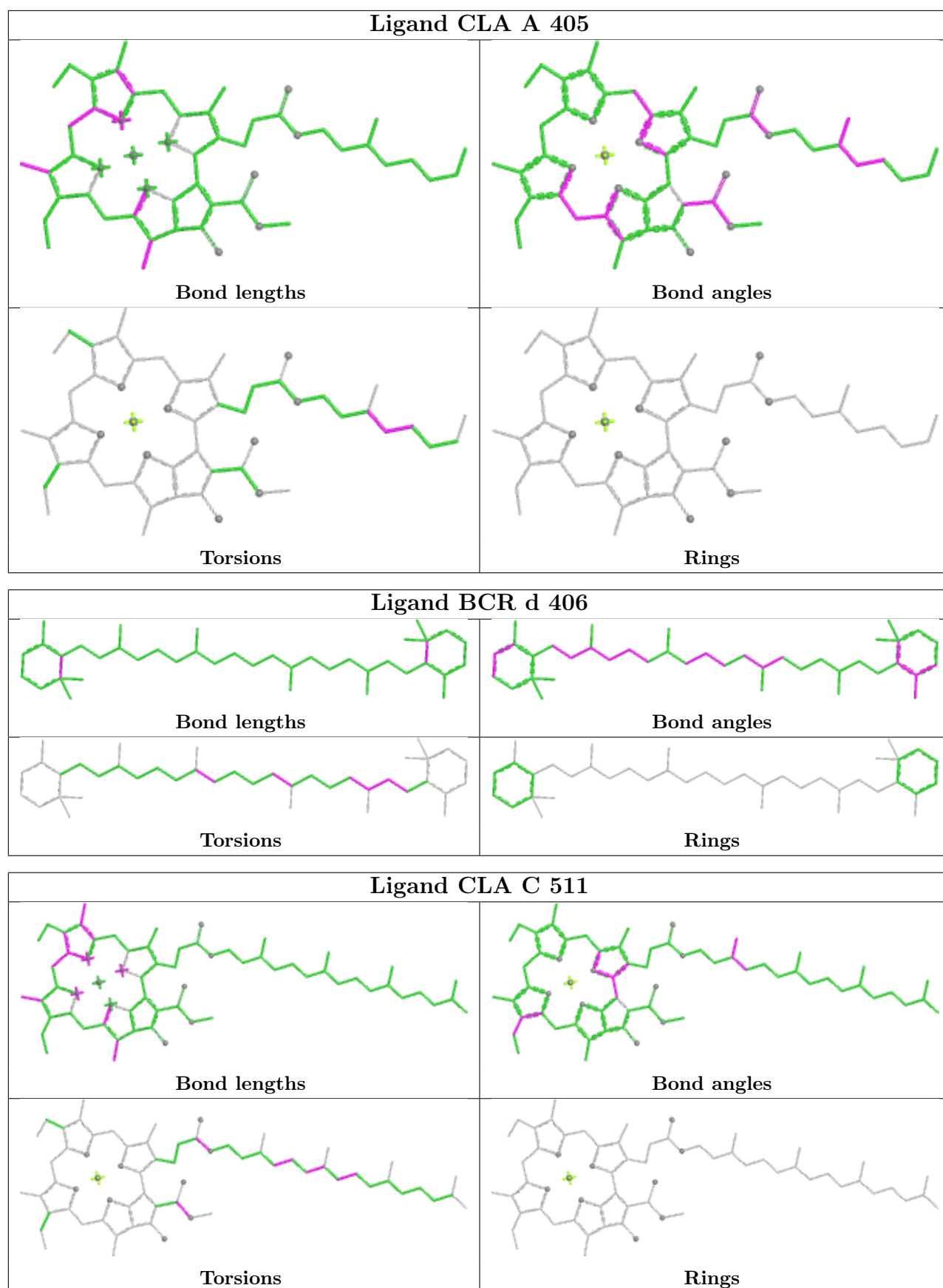
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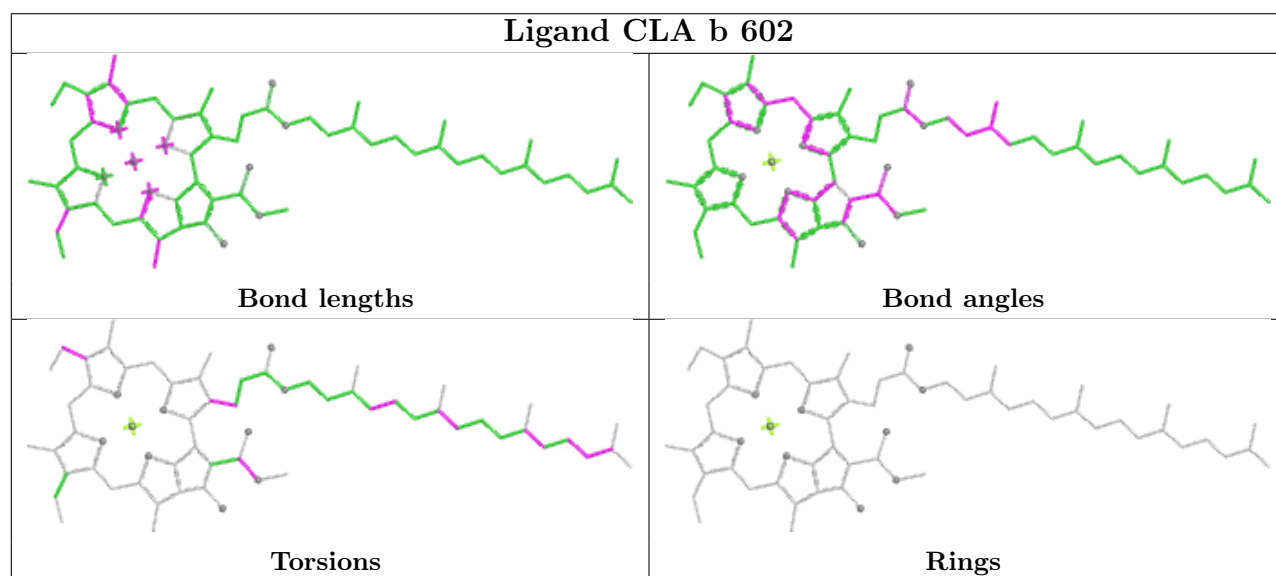
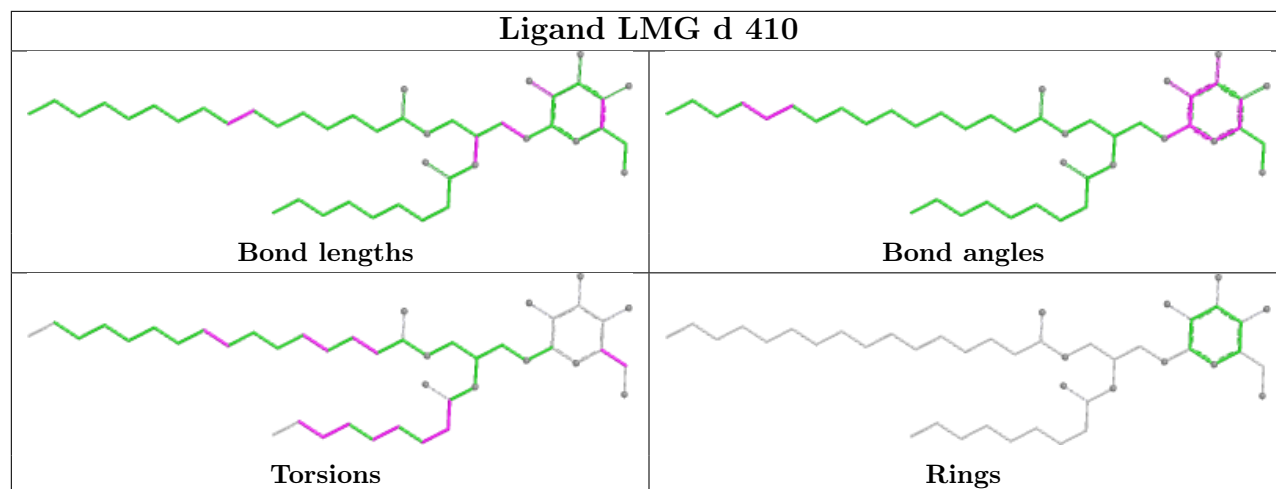


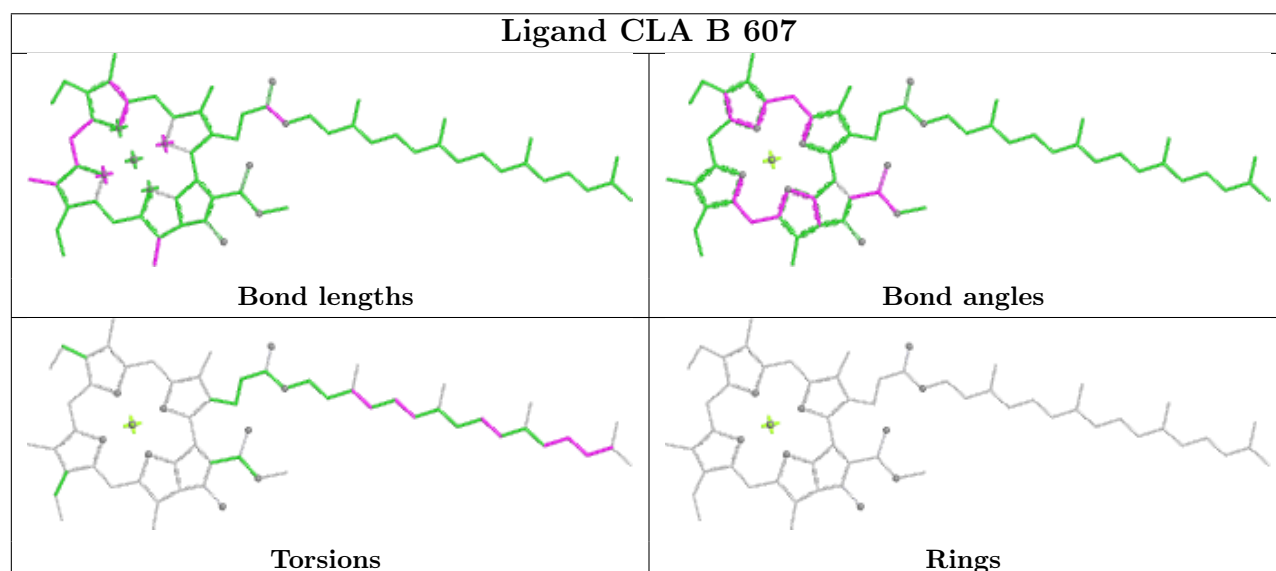
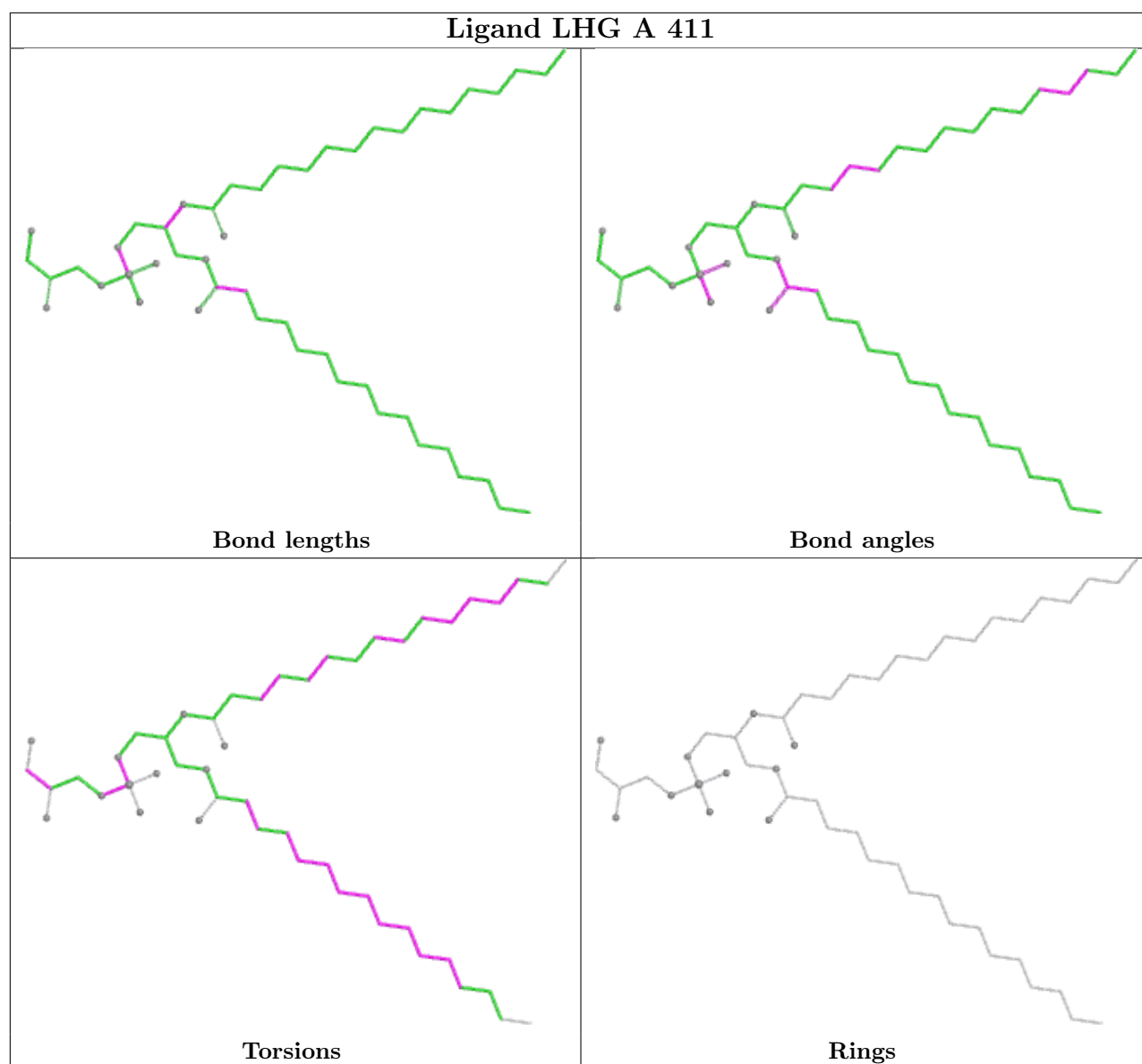
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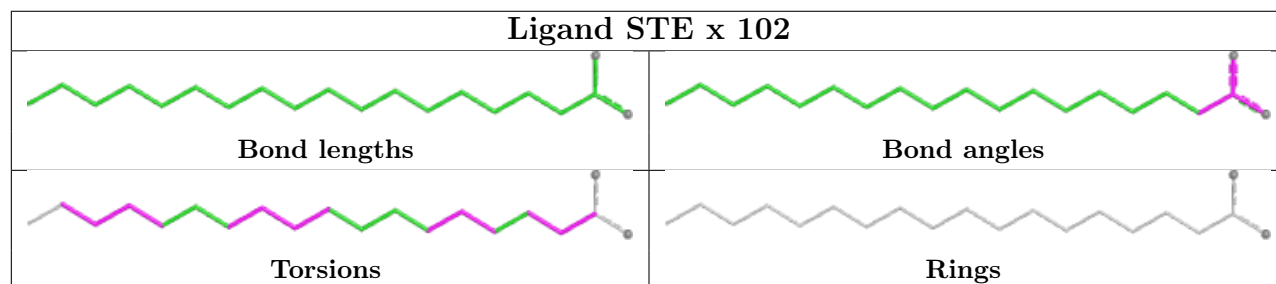
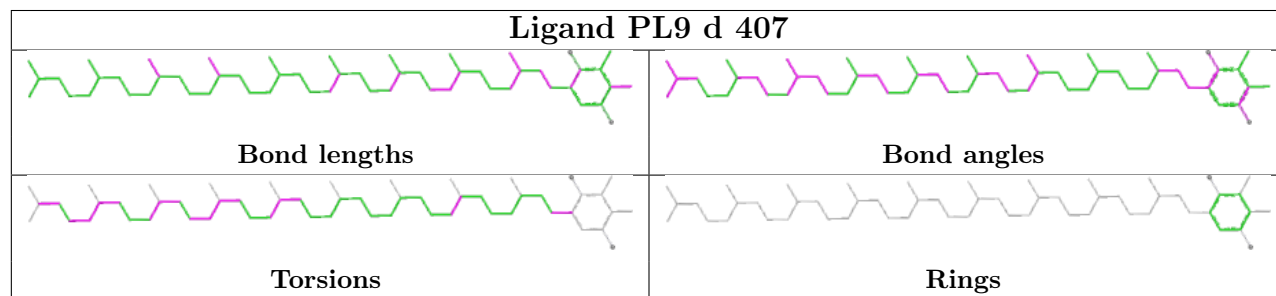
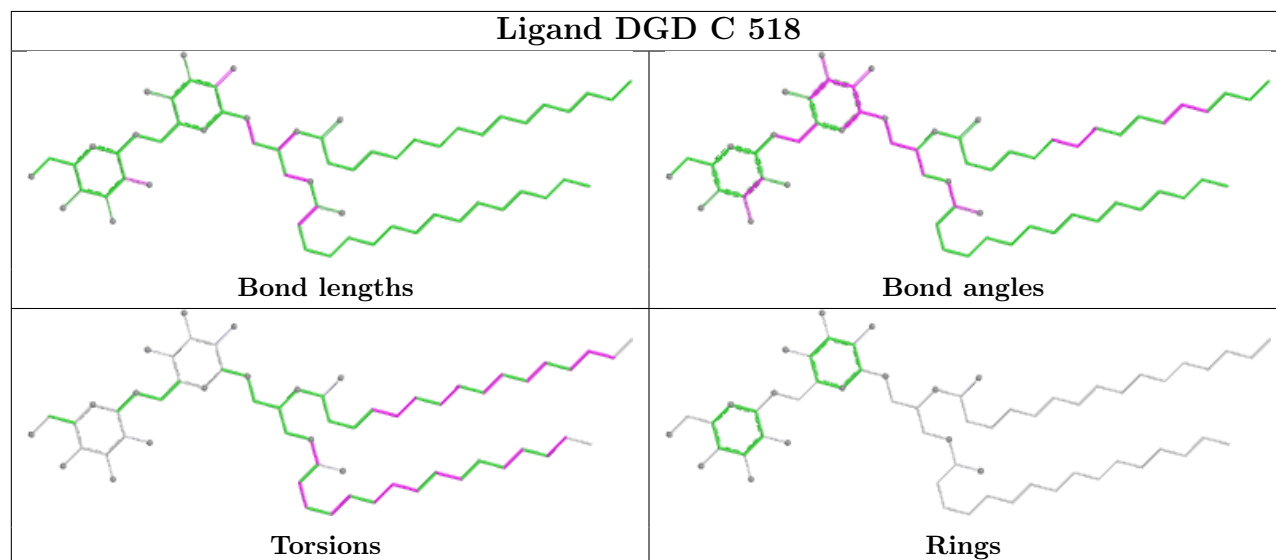
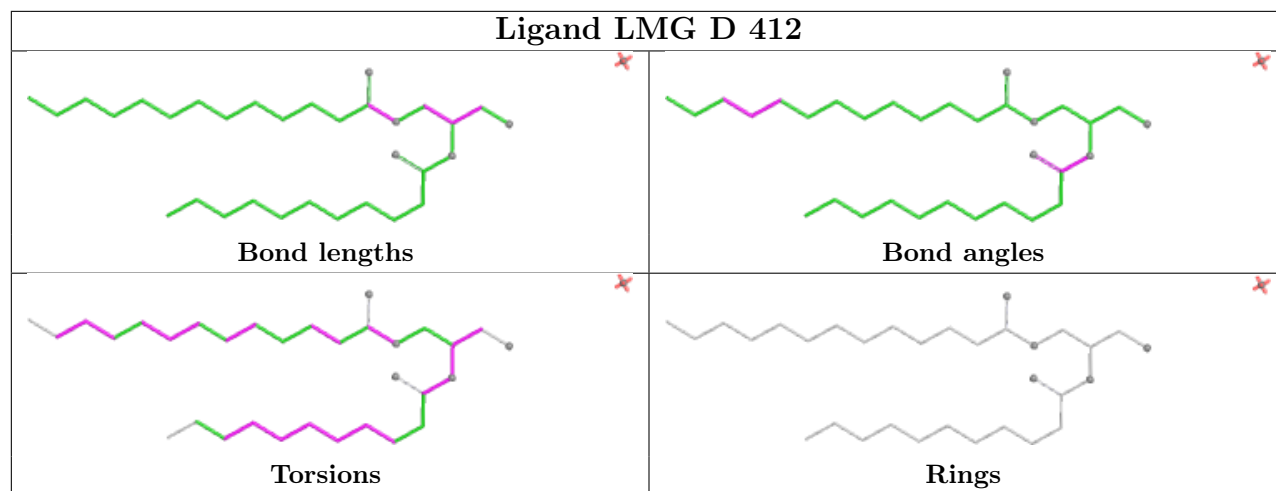


Ligand CLA B 603**Ligand CLA B 606****Ligand CLA b 614**

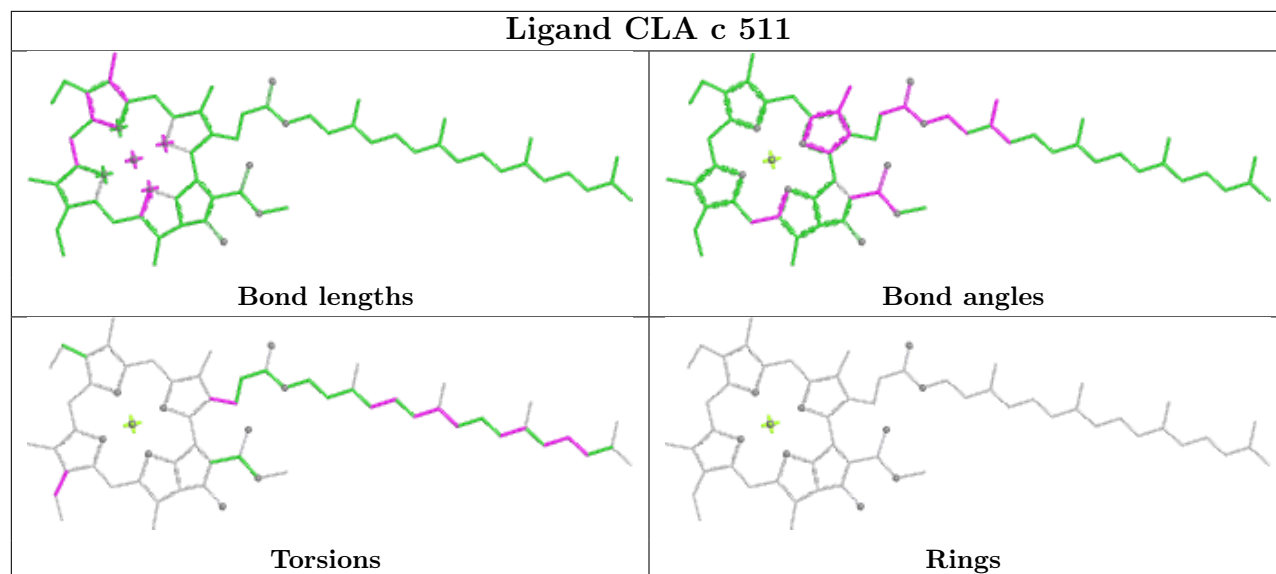




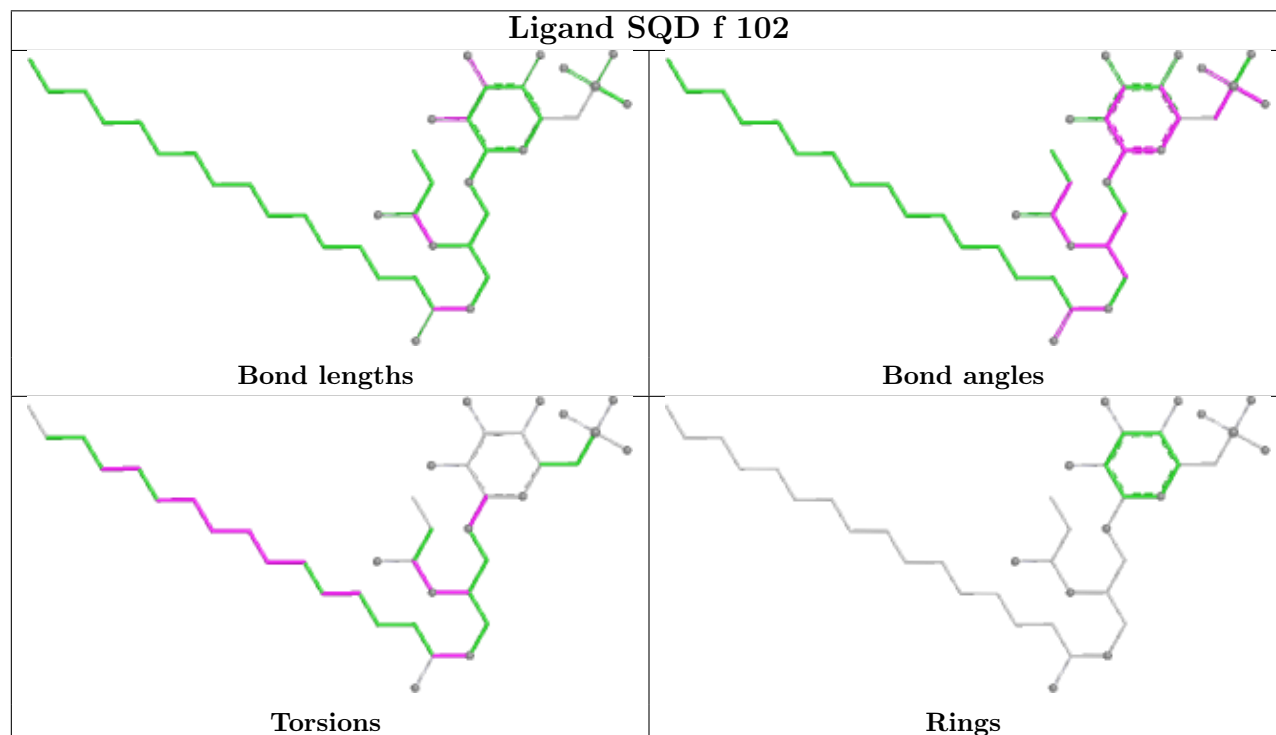




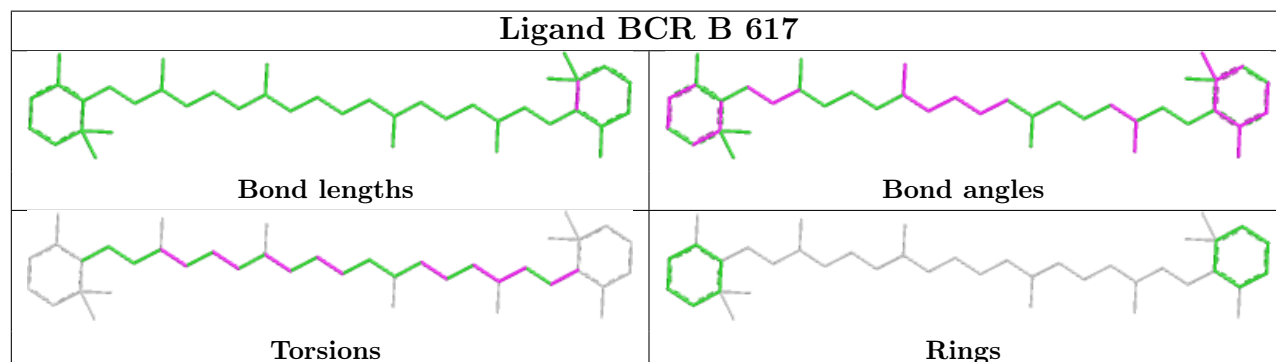
Ligand CLA c 511



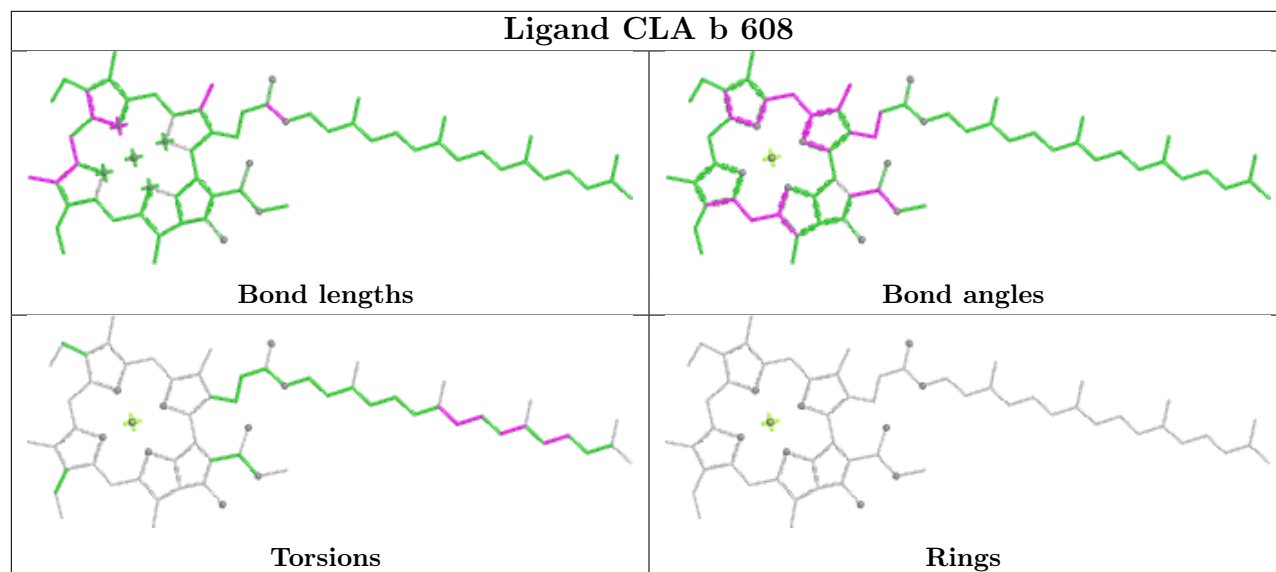
Ligand SQD f 102



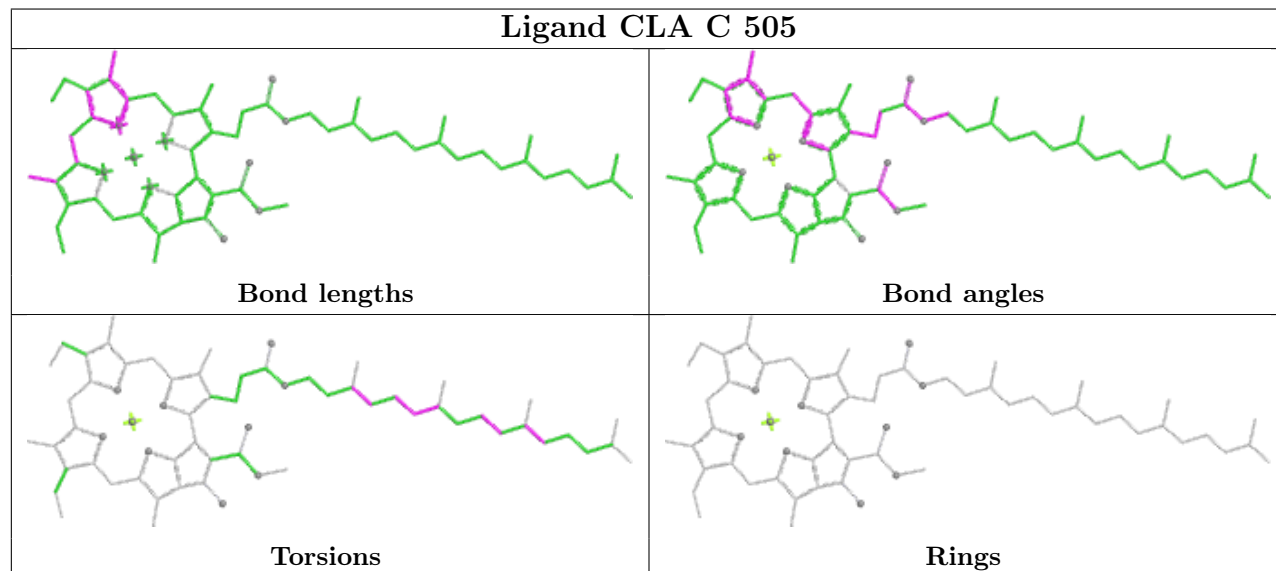
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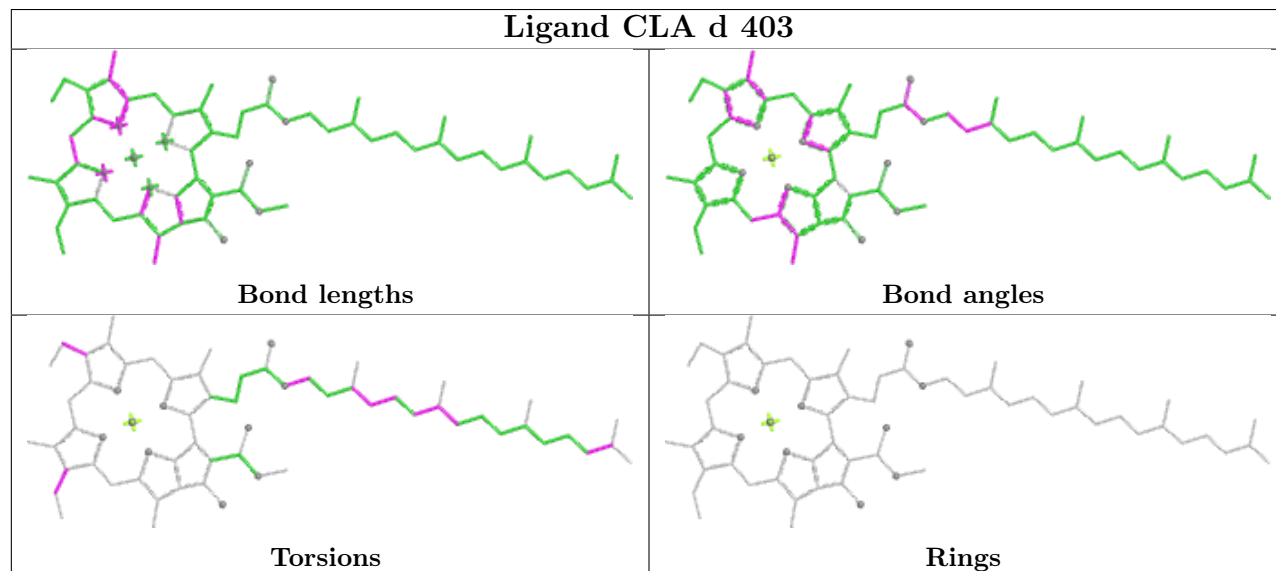
Ligand CLA b 608

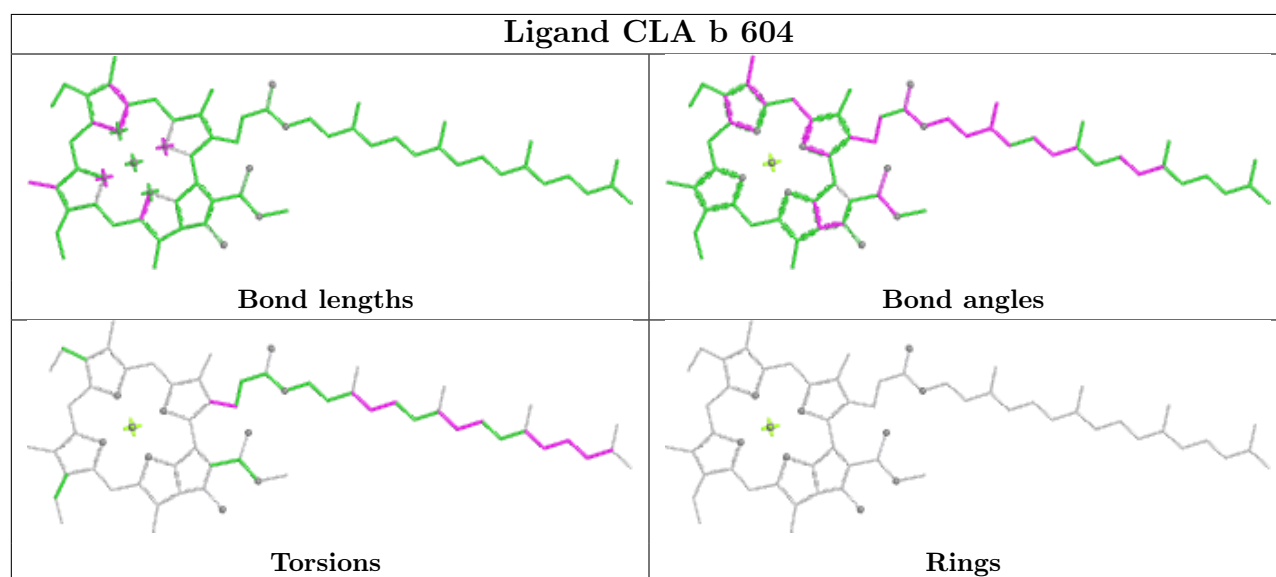
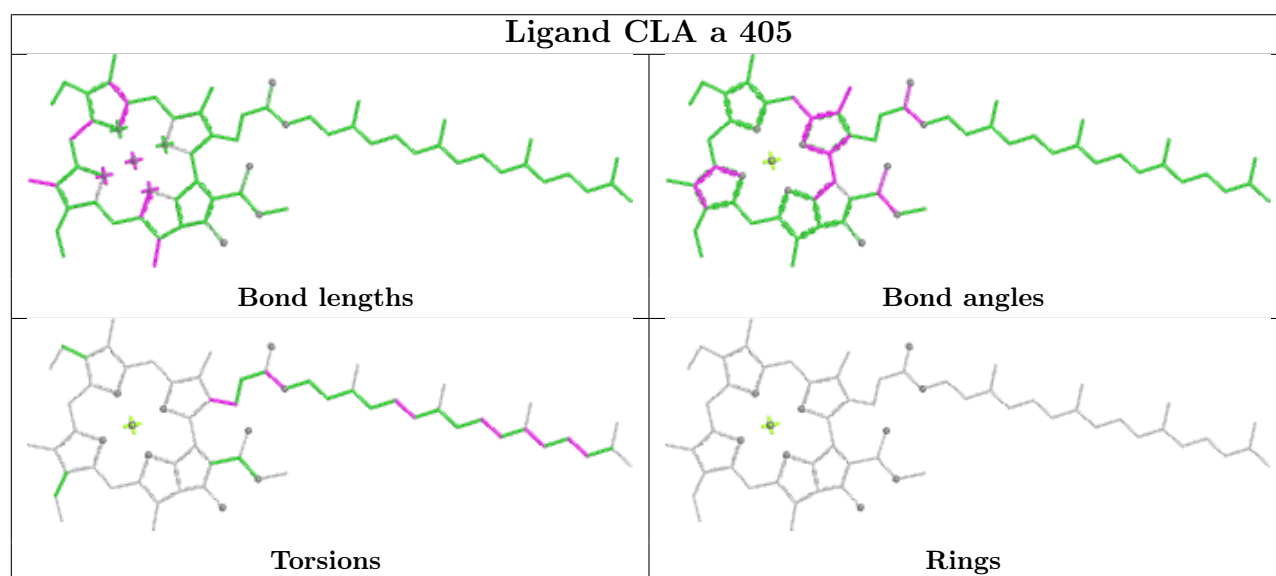
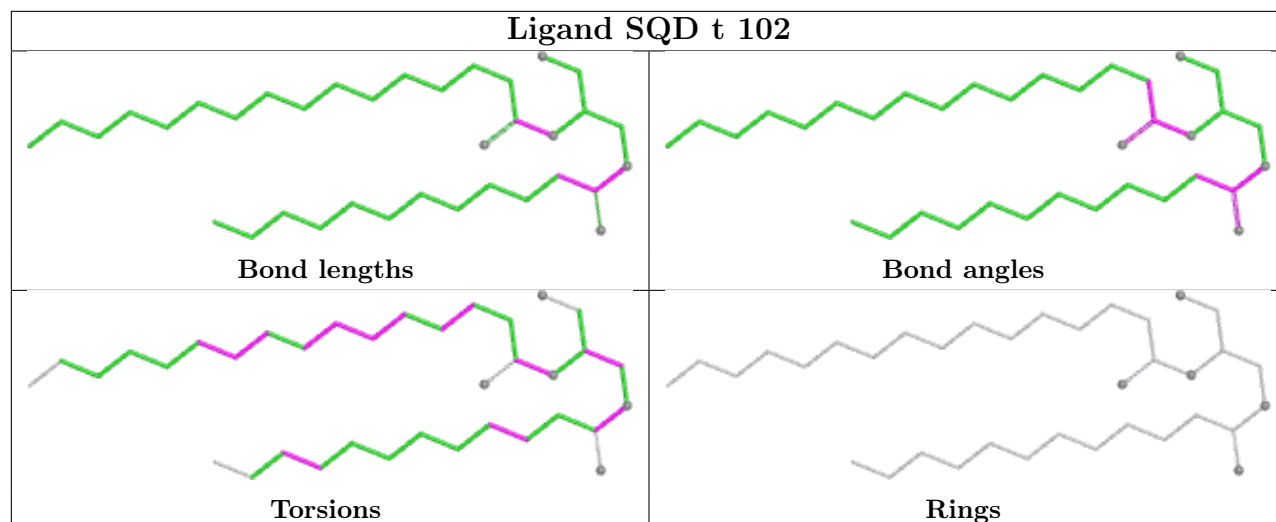


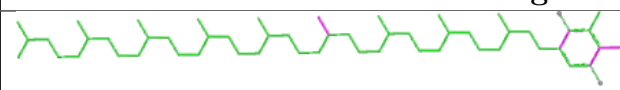
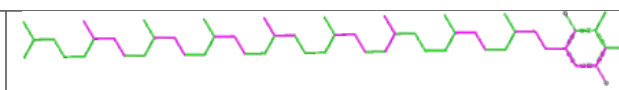
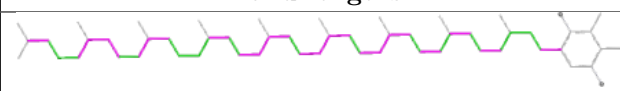
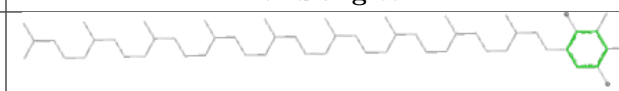
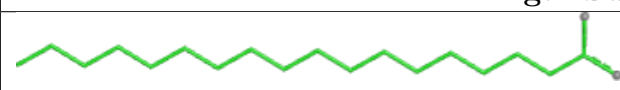
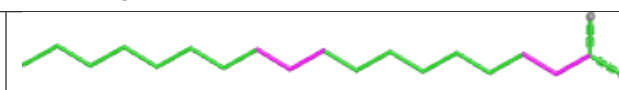
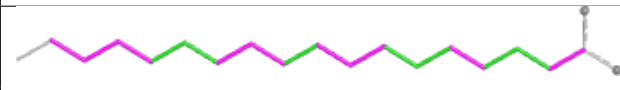
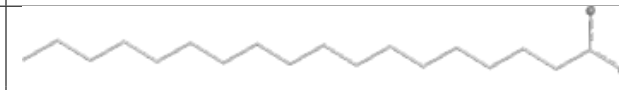
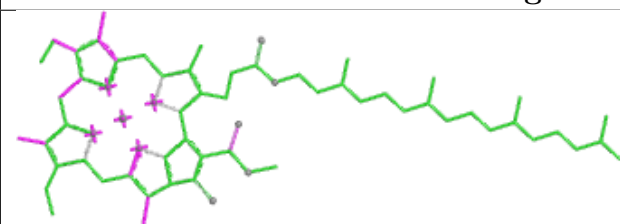
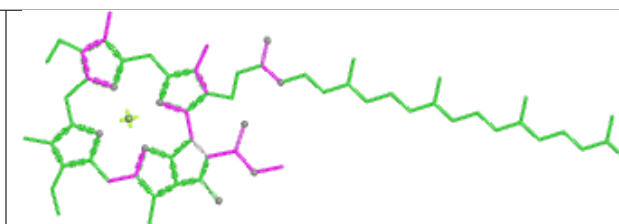
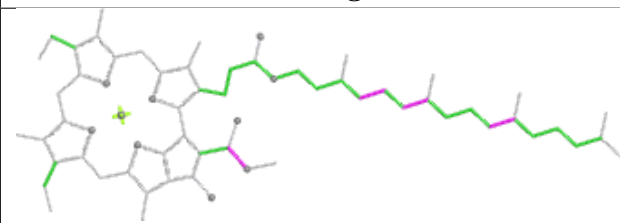
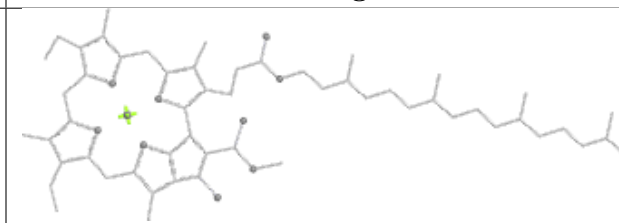
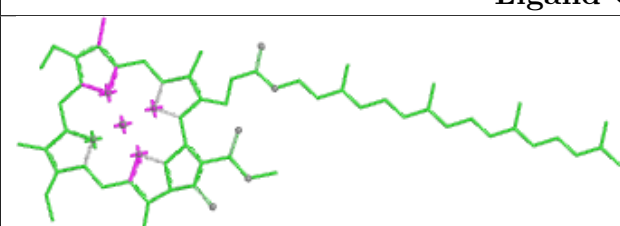
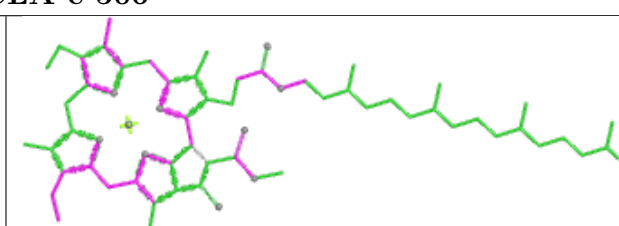
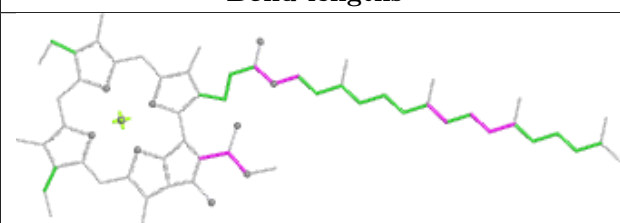
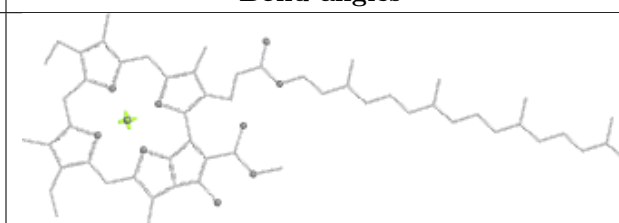
Ligand CLA C 505

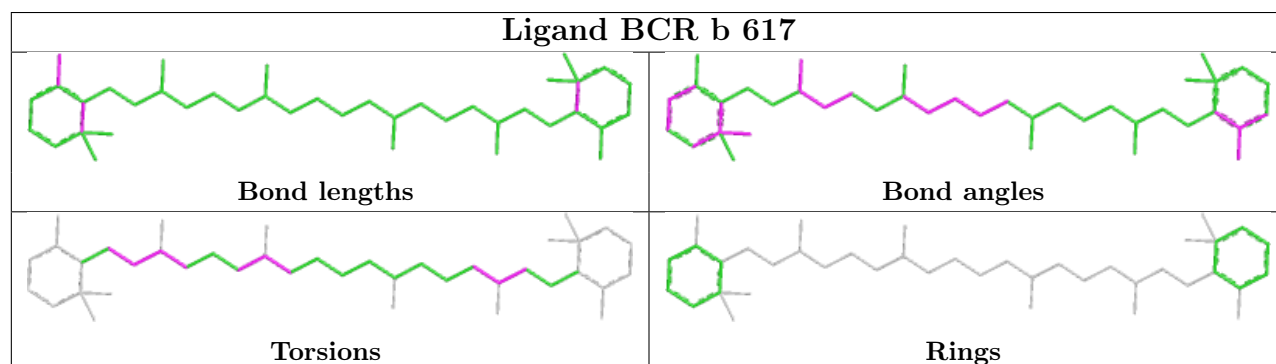
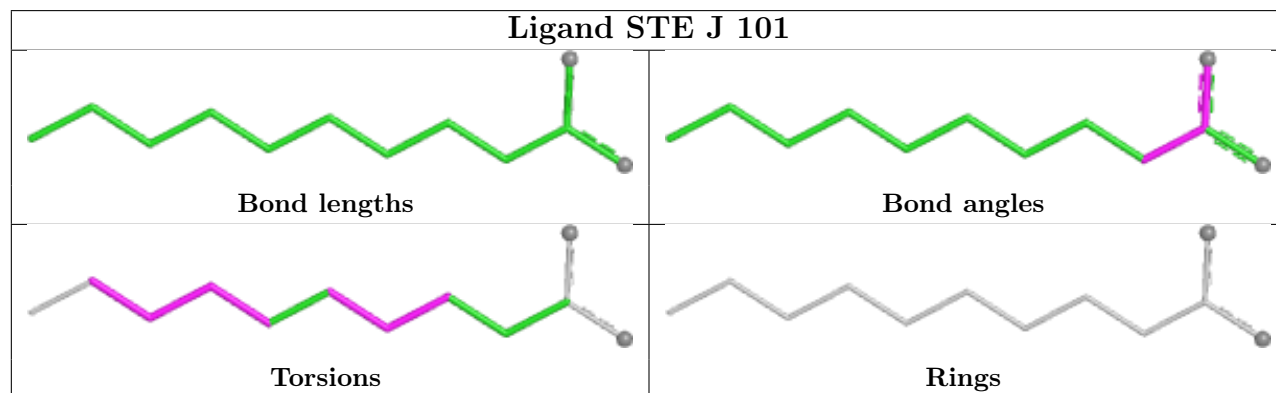
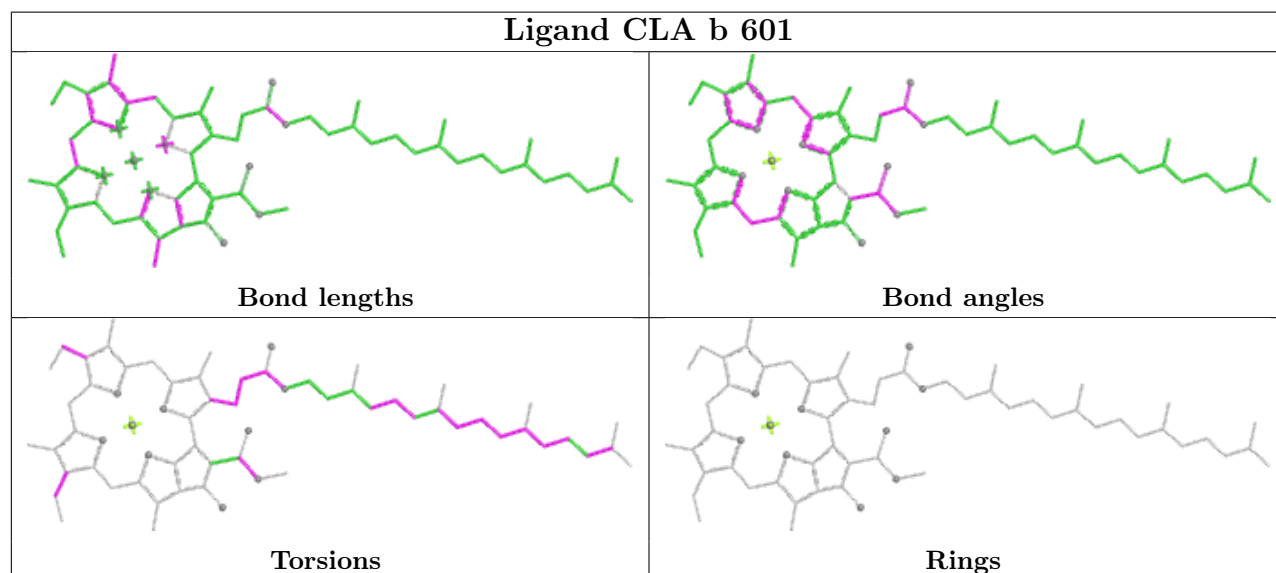
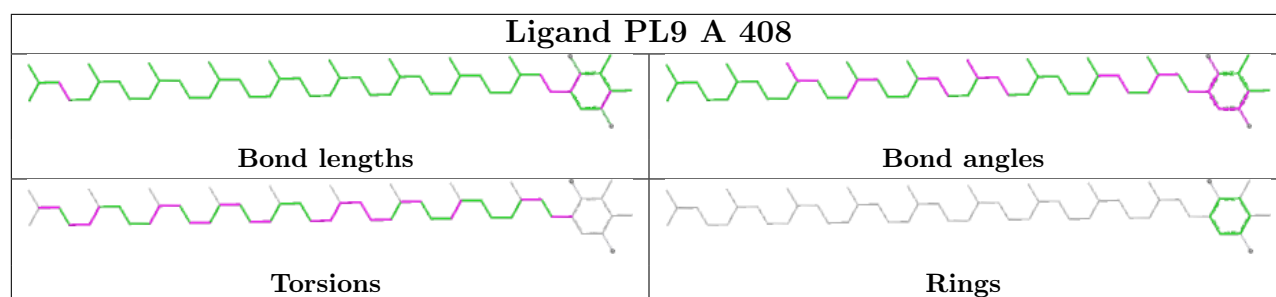


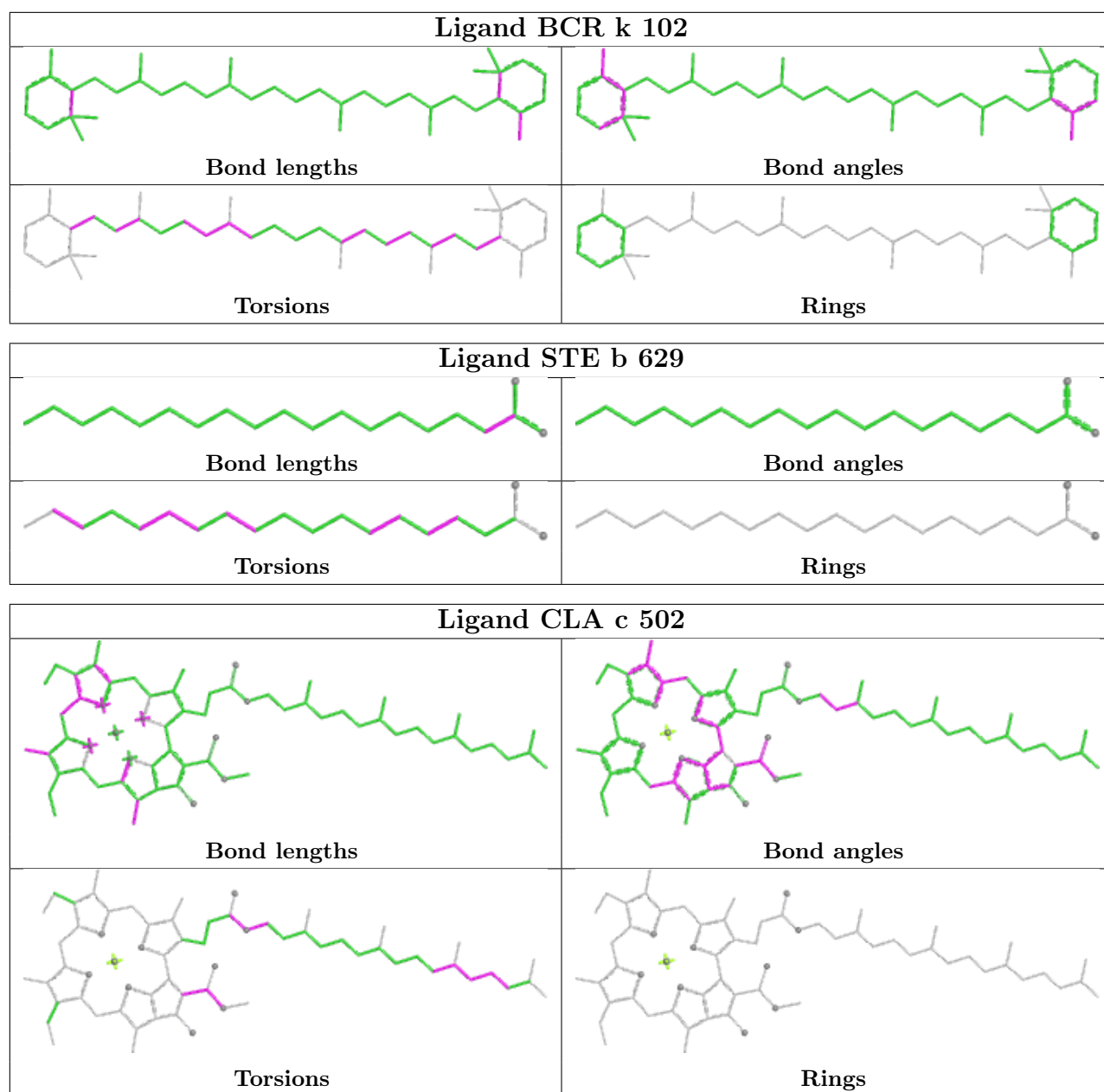
Ligand CLA d 403



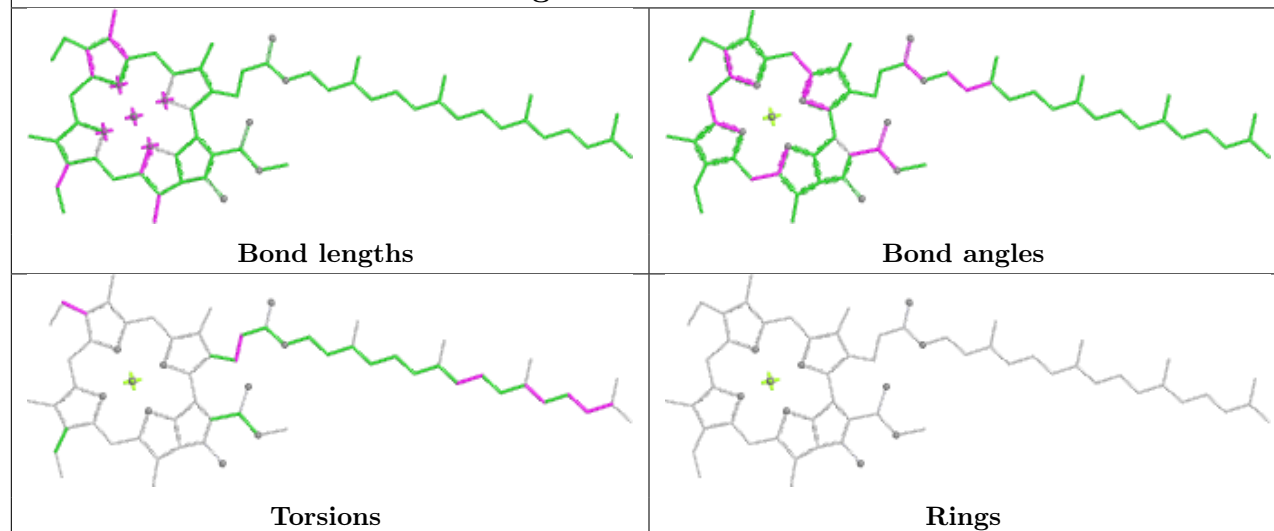


Ligand PL9 a 409	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE X 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA c 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

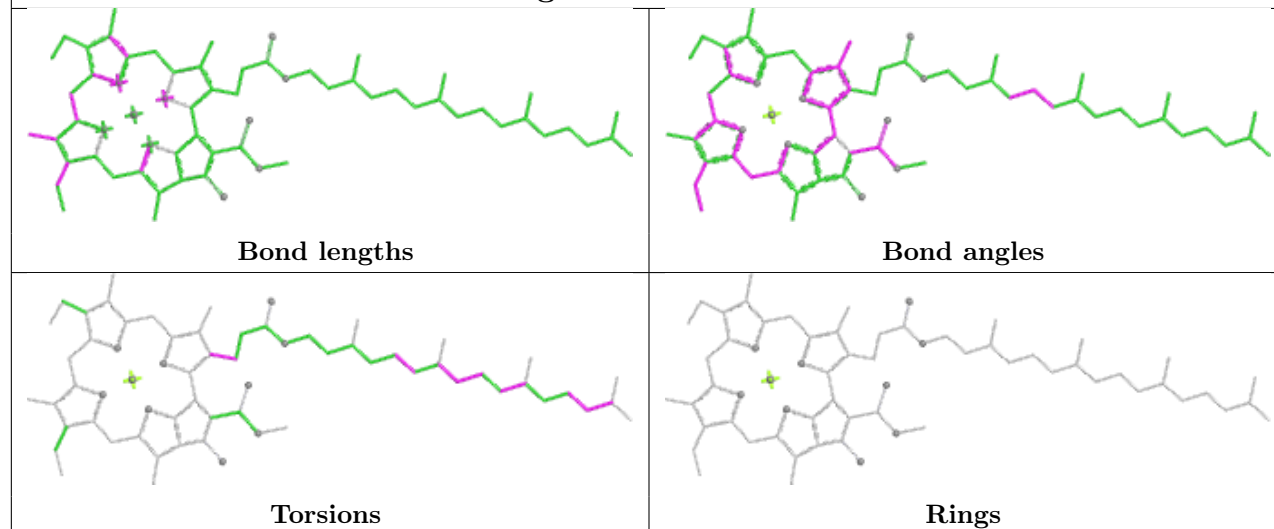




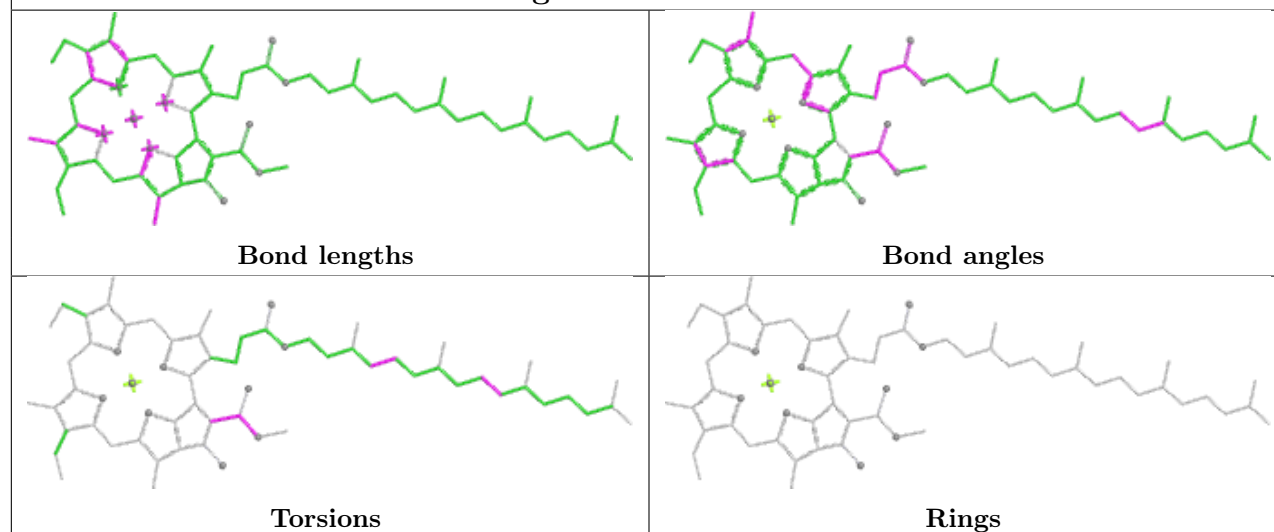
Ligand CLA B 609

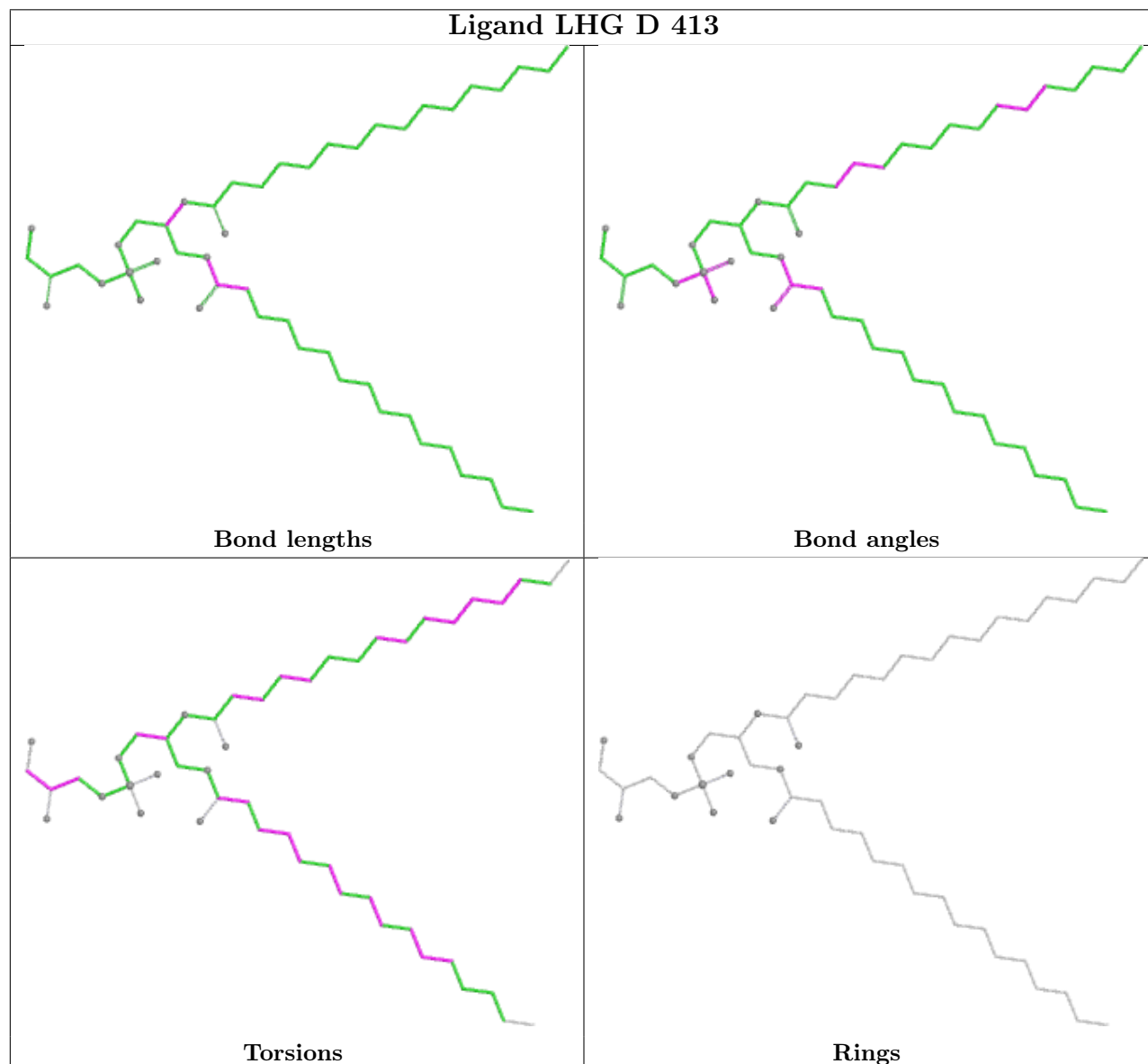
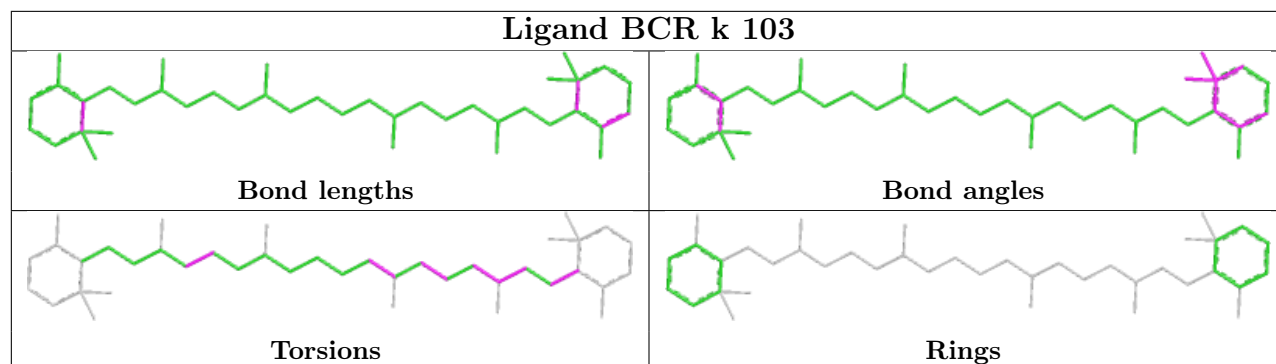


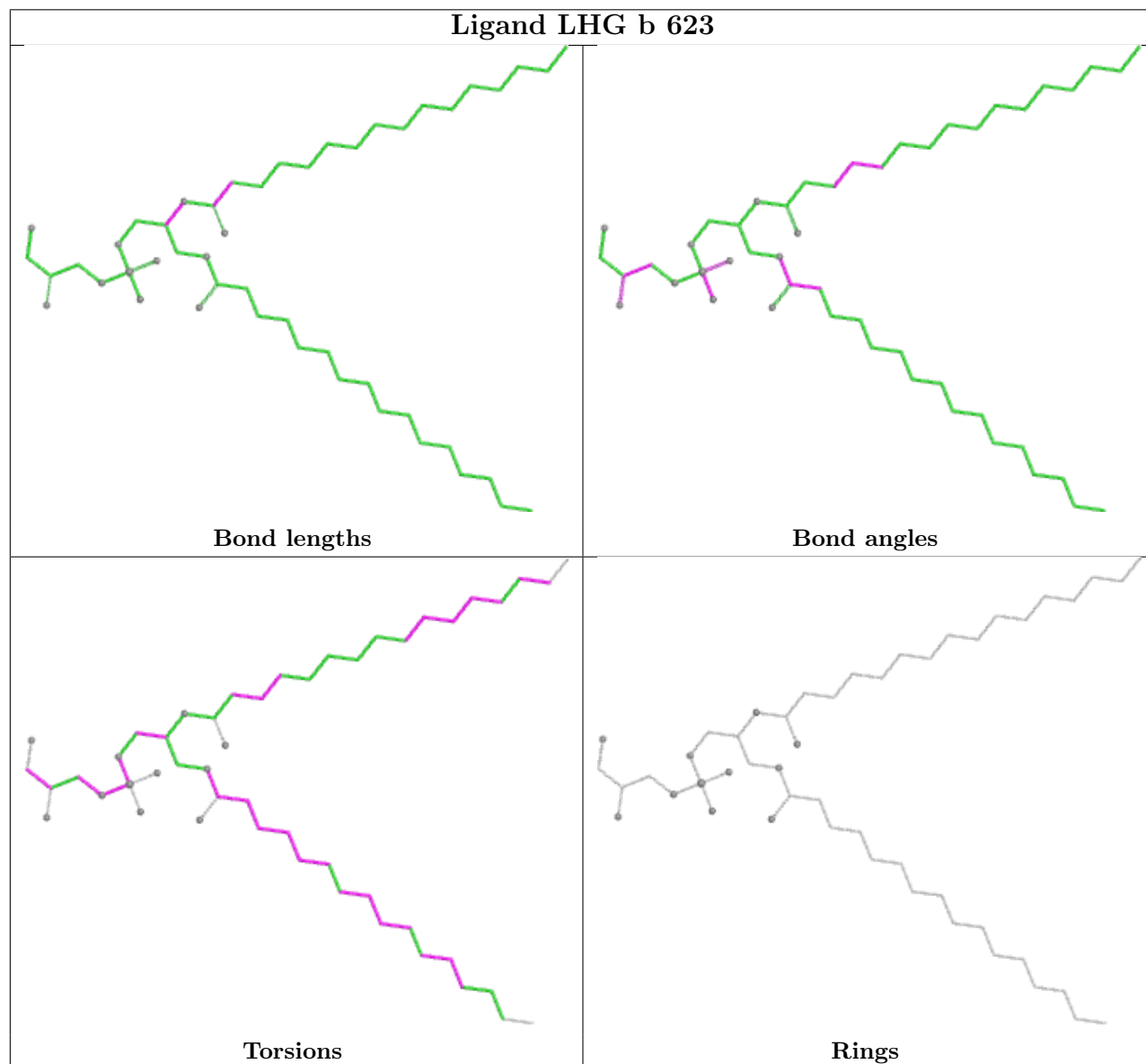
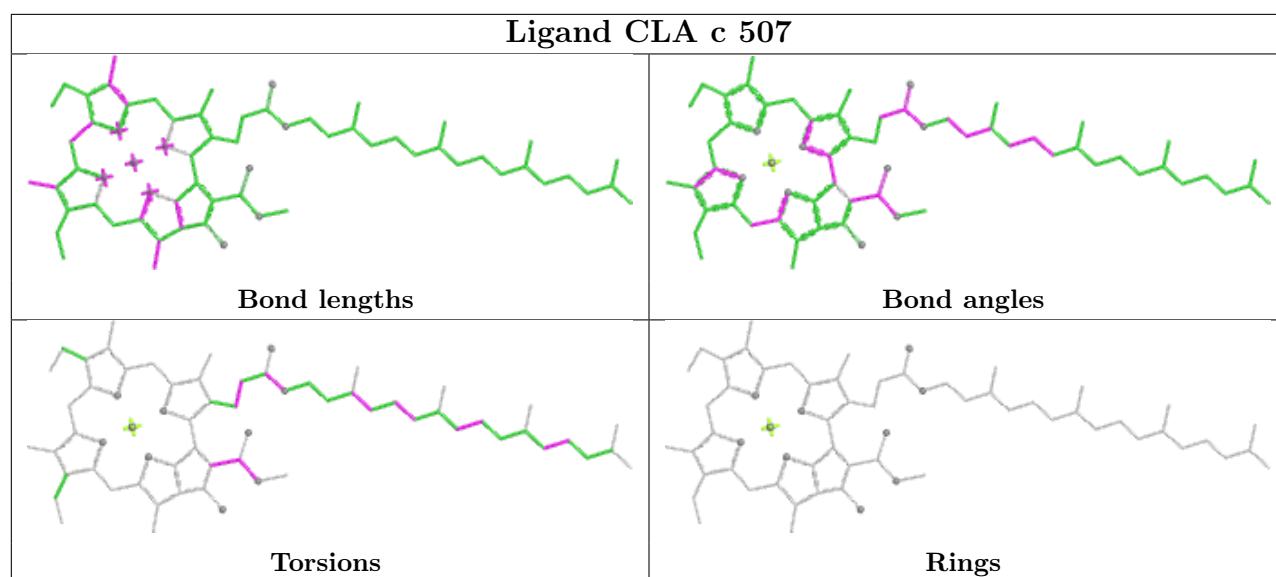
Ligand CLA c 503

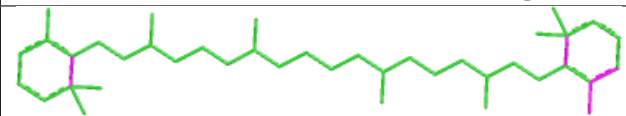
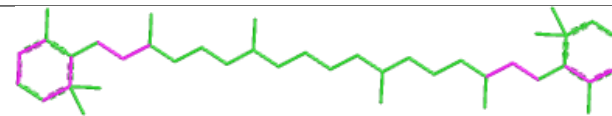
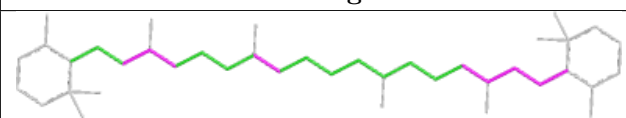
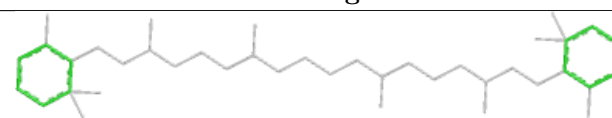


Ligand CLA B 611

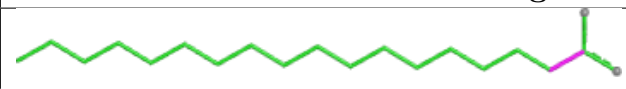
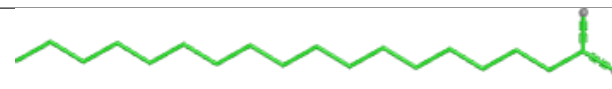
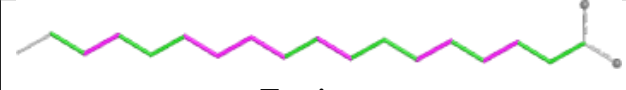
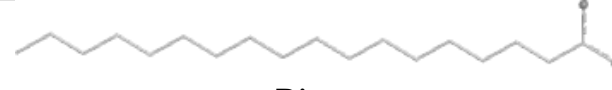


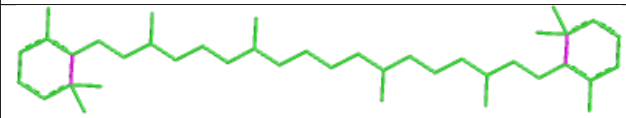
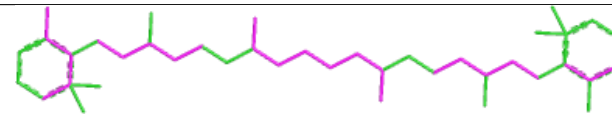
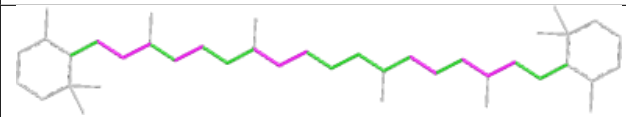
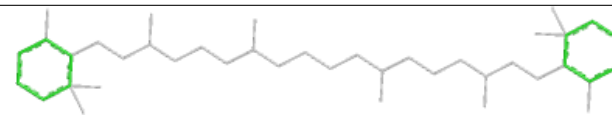


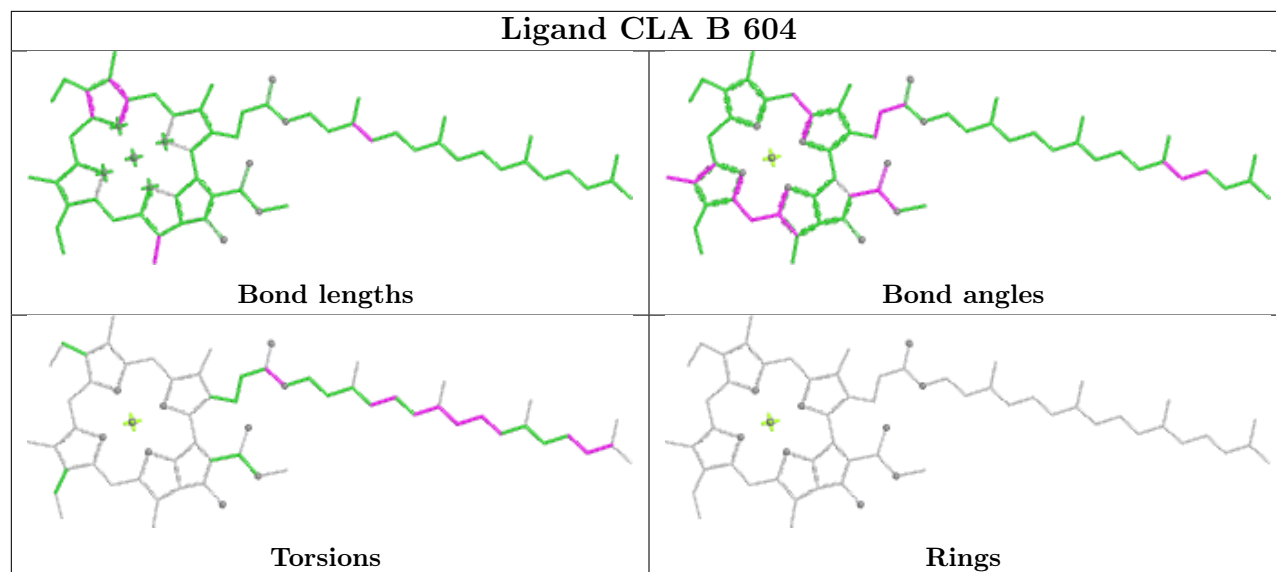
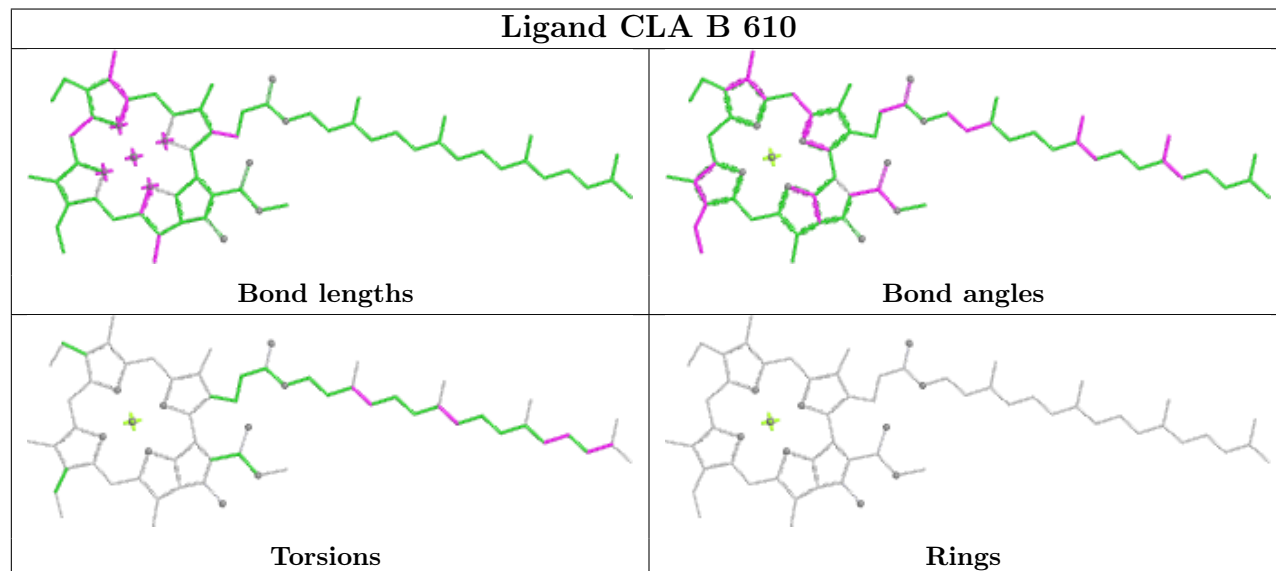


Ligand BCR D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

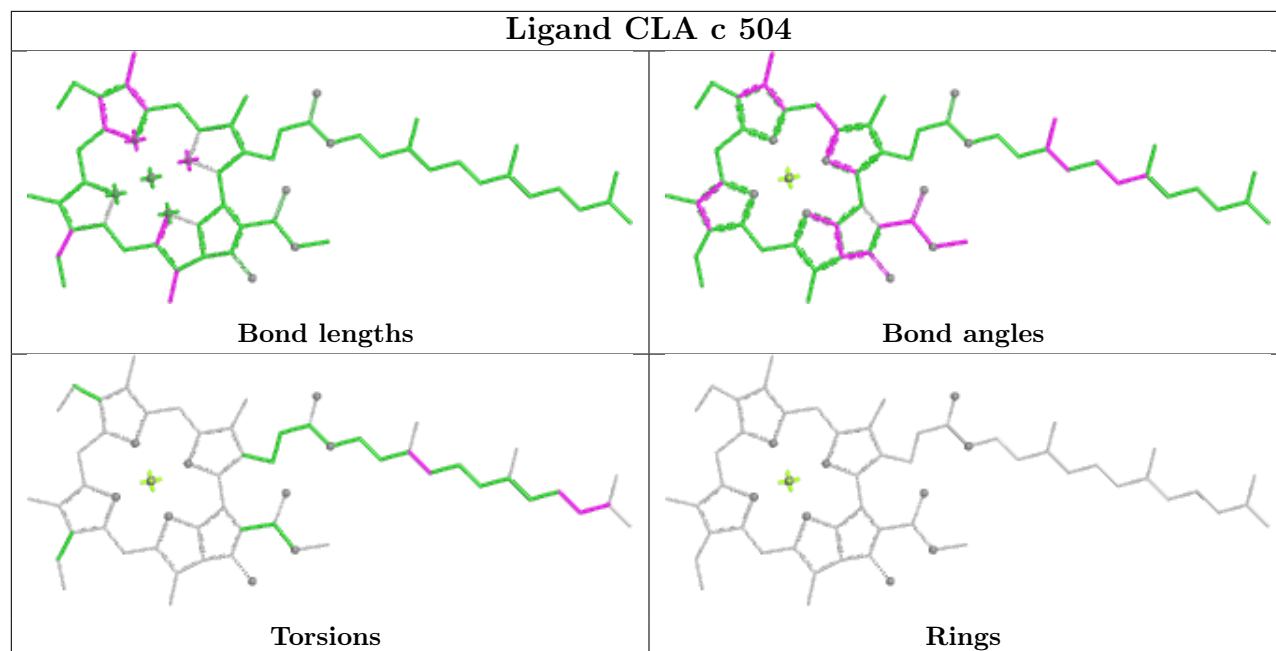
Ligand STE B 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE c 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

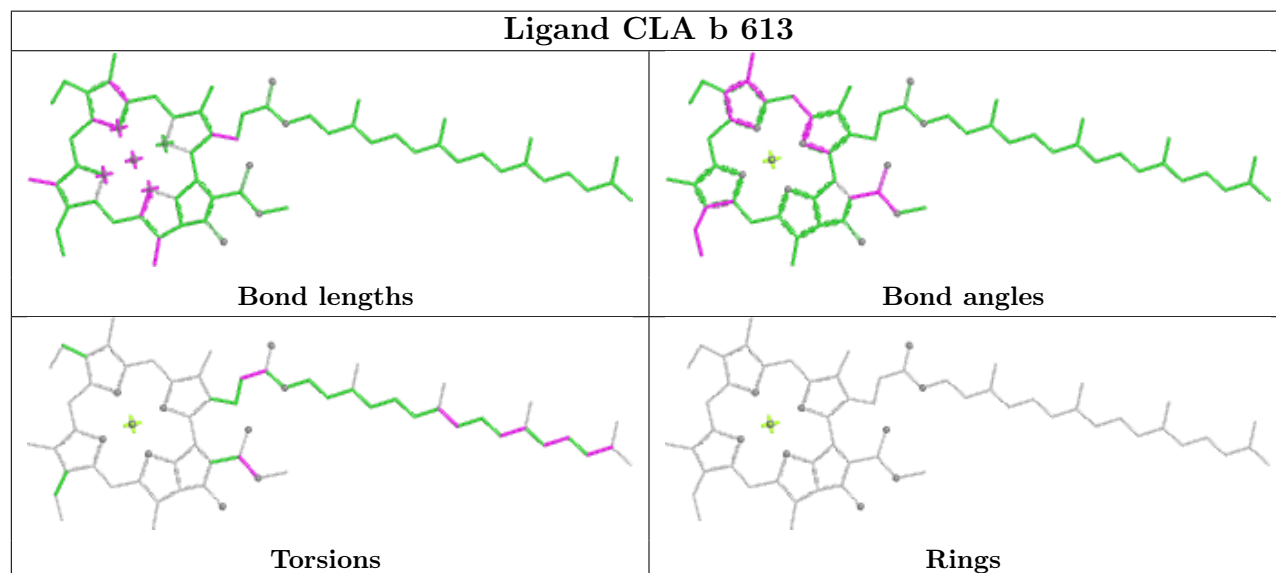
Ligand BCR k 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

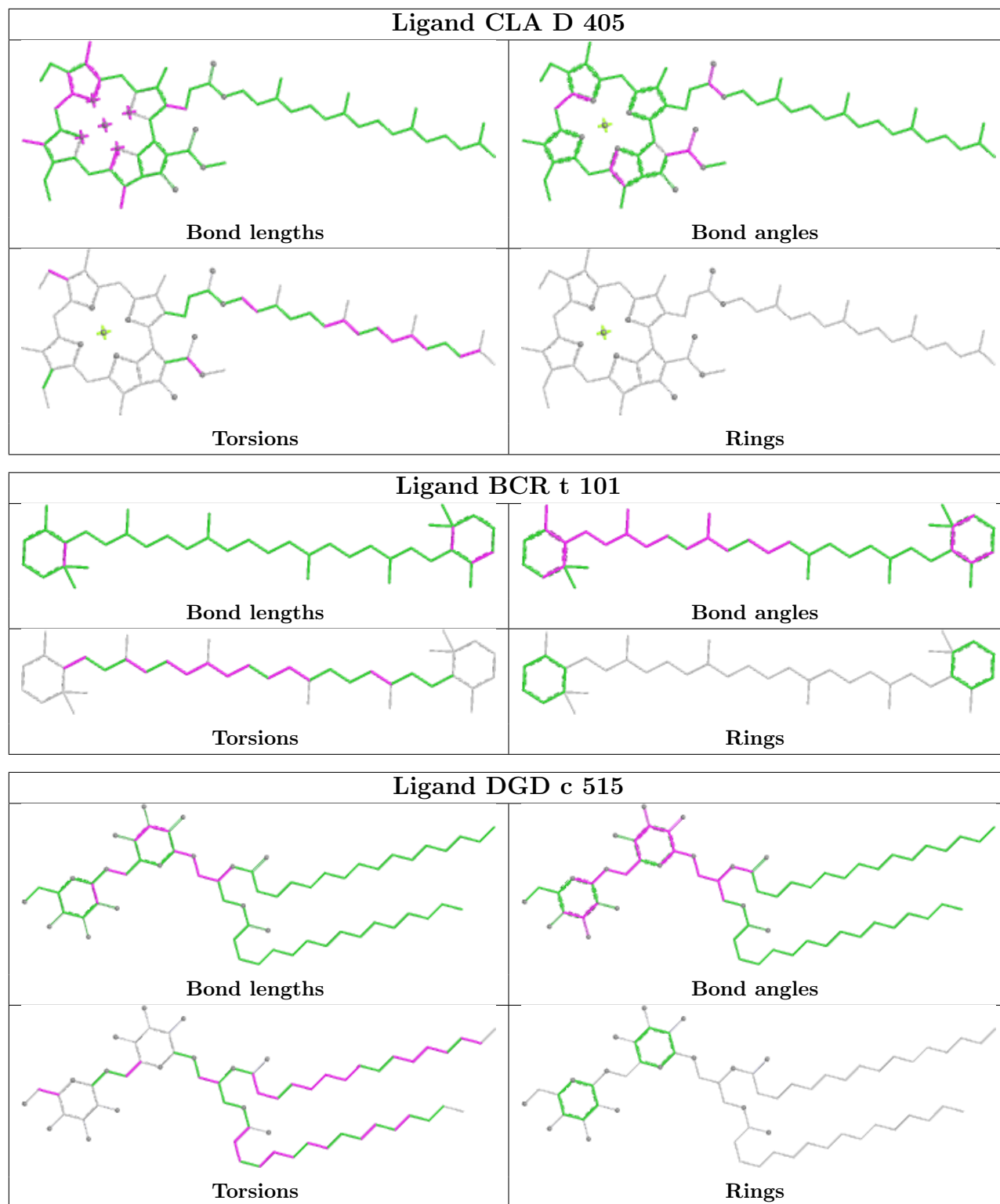
Ligand CLA B 604**Ligand CLA B 610**

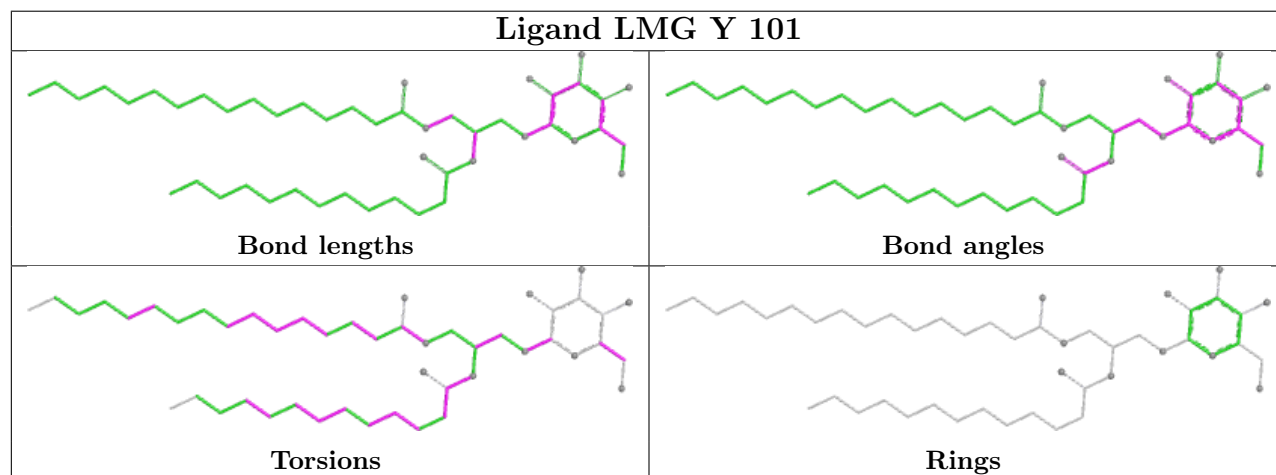
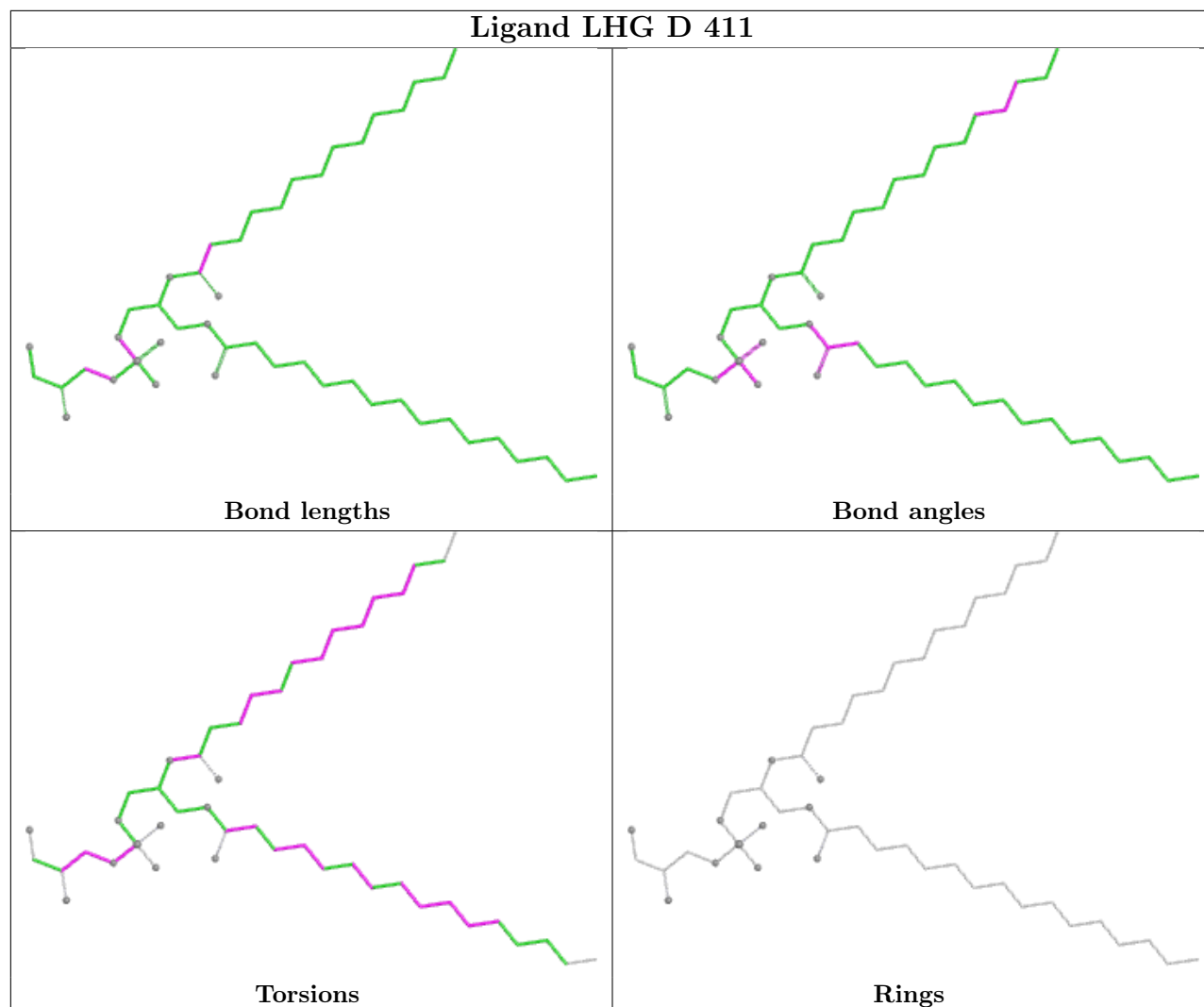
Ligand CLA c 504

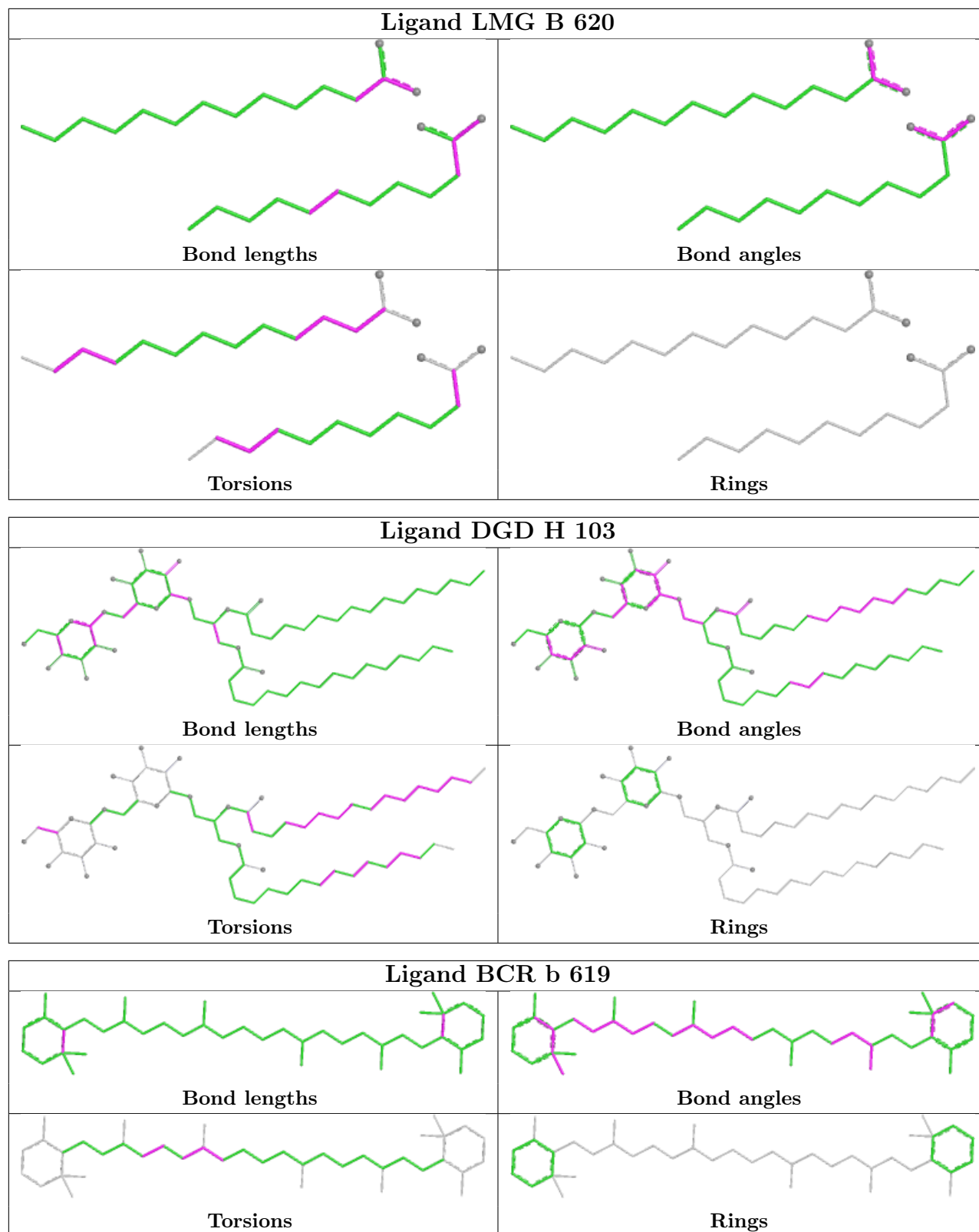


Ligand CLA b 613

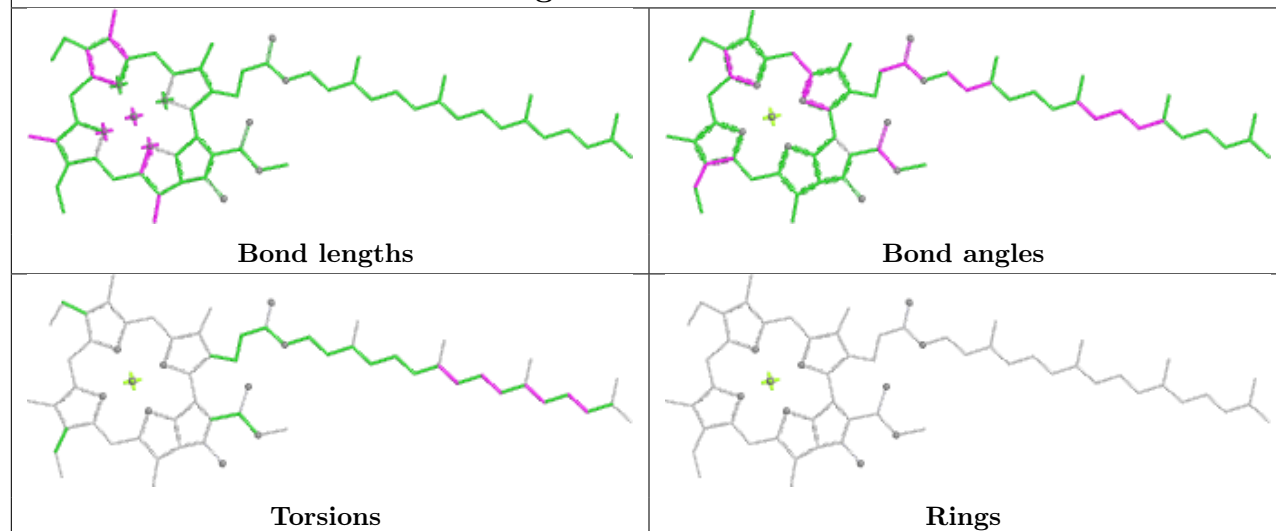




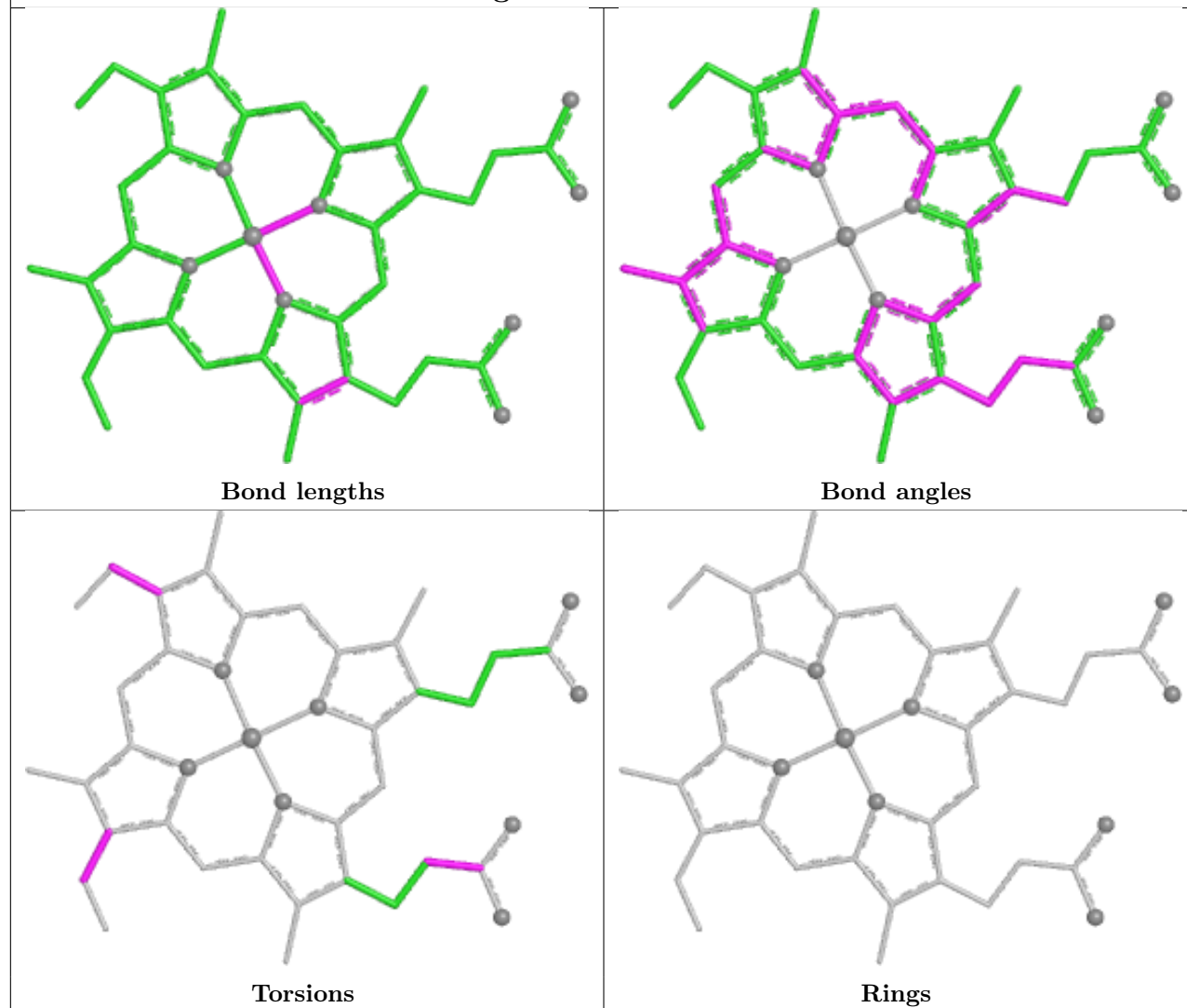


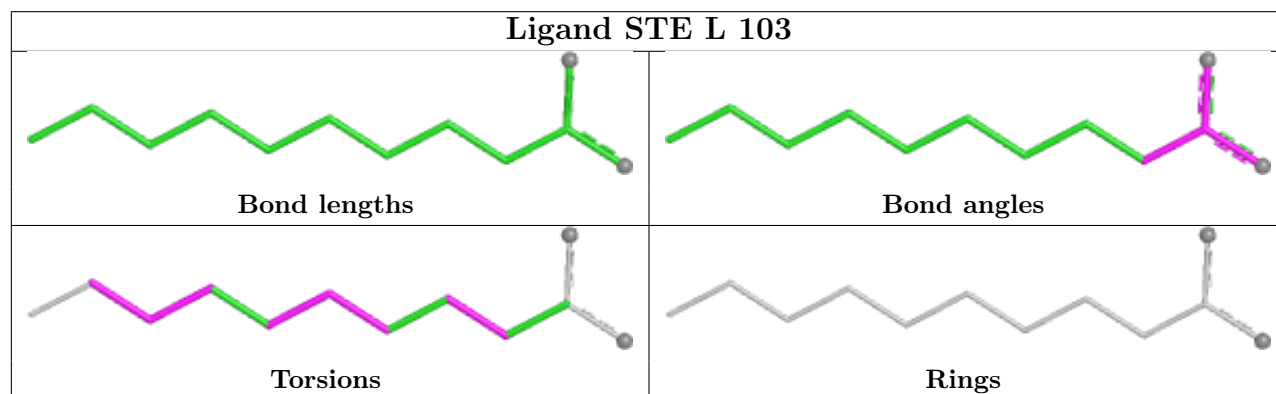
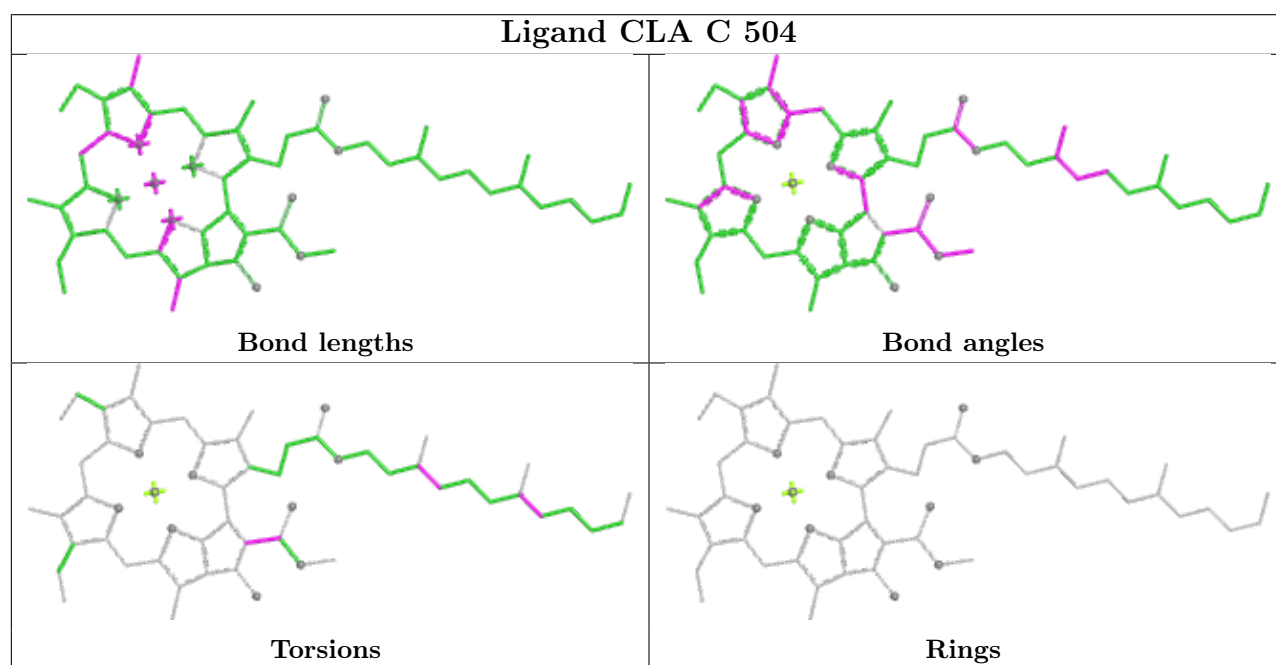
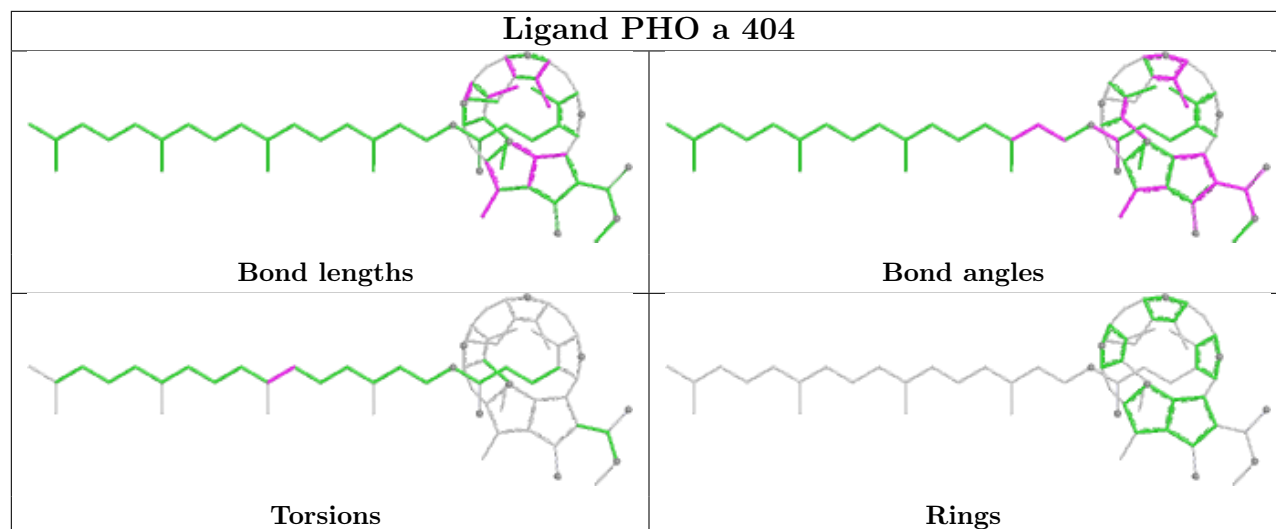


Ligand CLA b 612

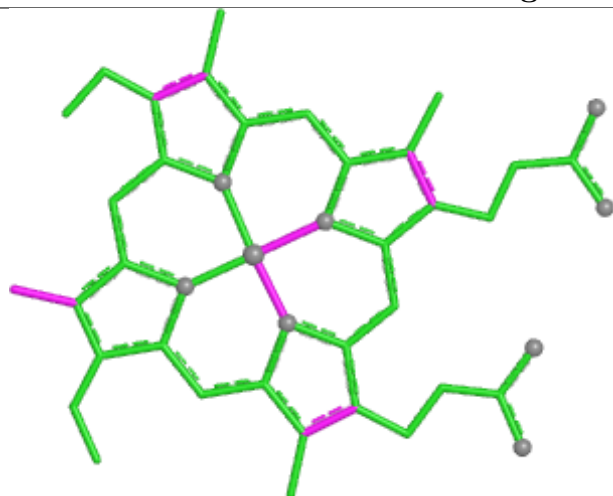


Ligand HEC V 201

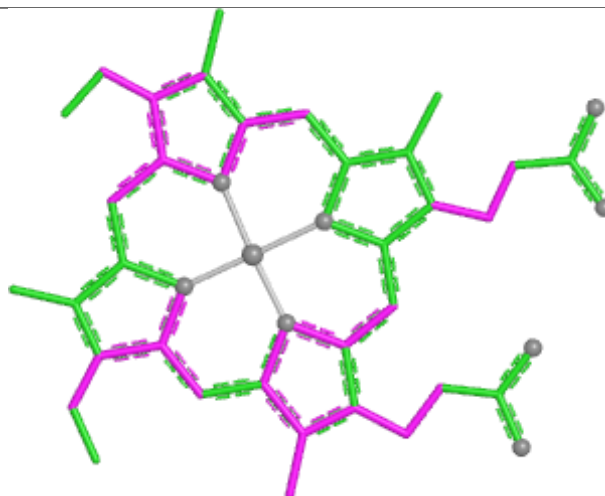




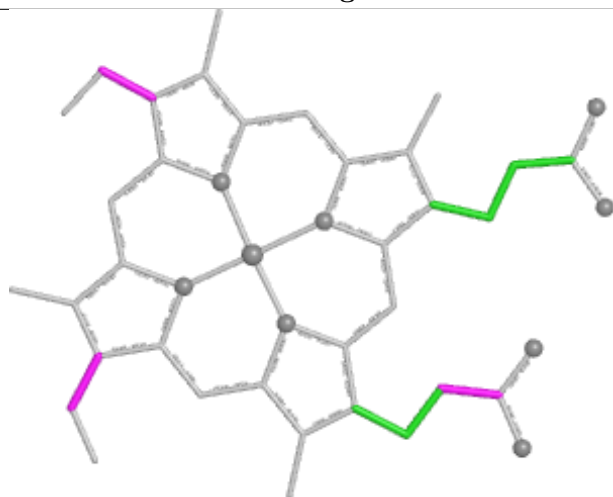
Ligand HEC f 101



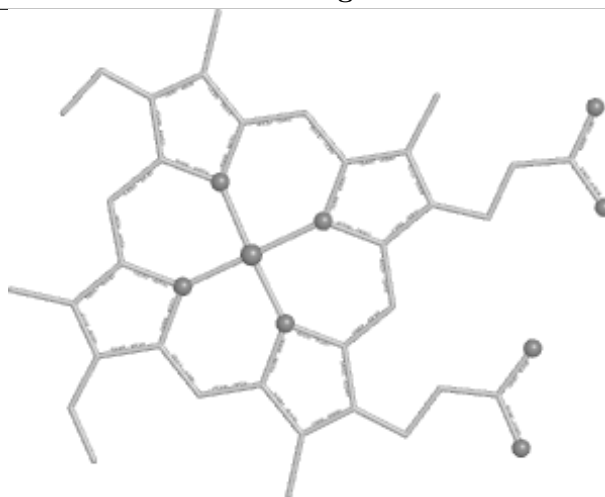
Bond lengths



Bond angles

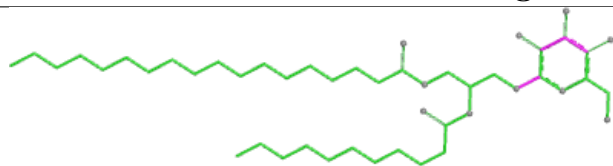


Torsions

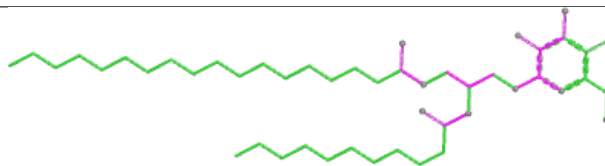


Rings

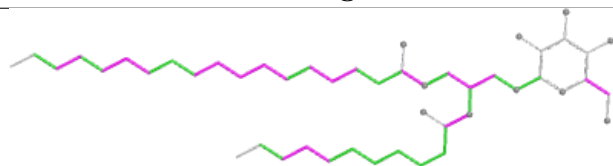
Ligand LMG c 520



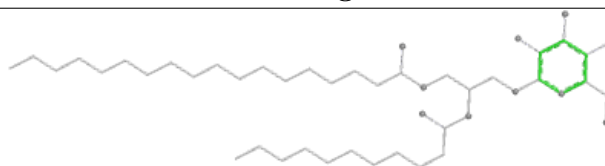
Bond lengths



Bond angles

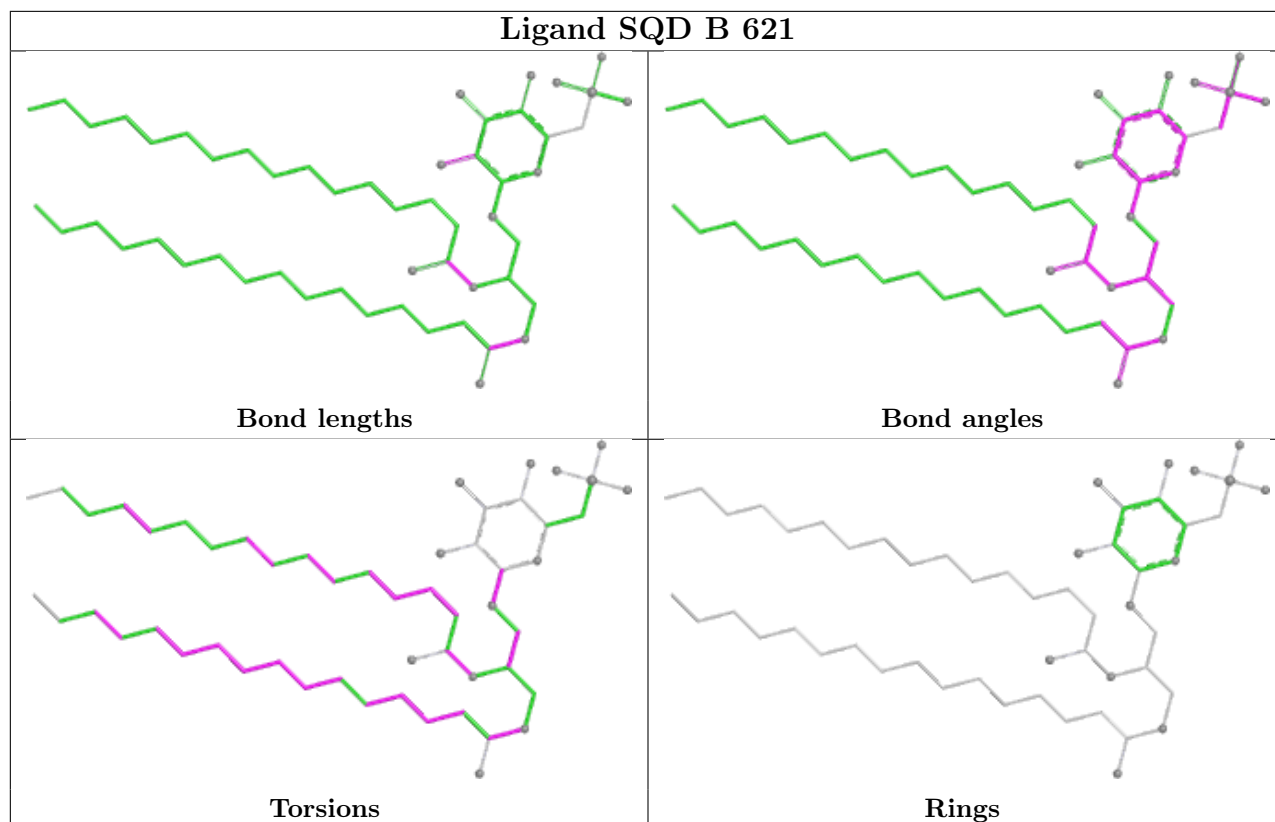


Torsions

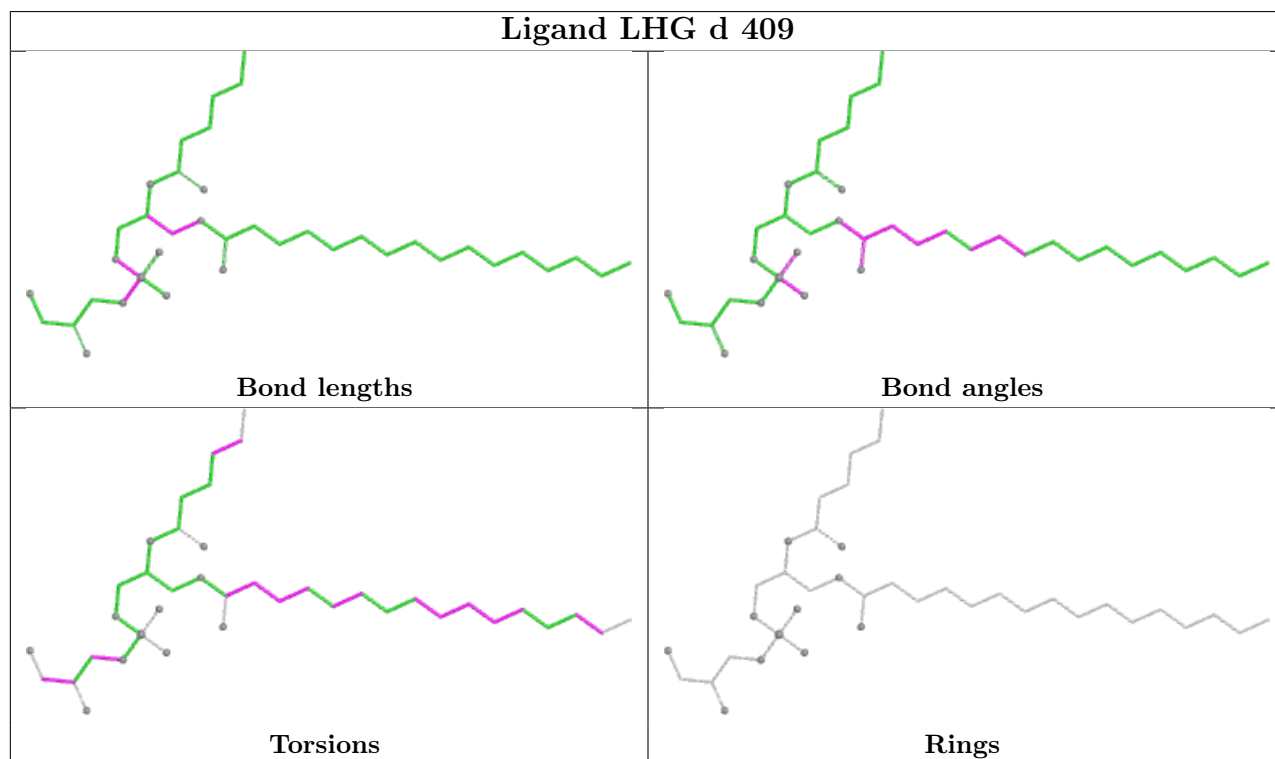


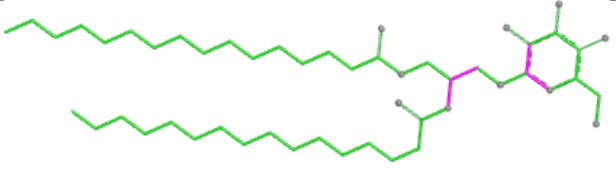
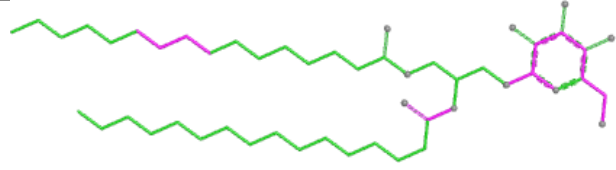
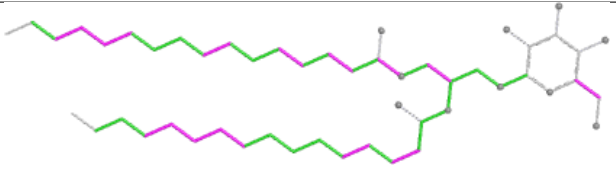
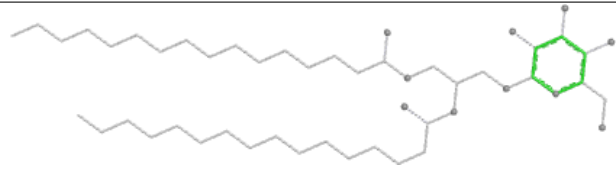
Rings

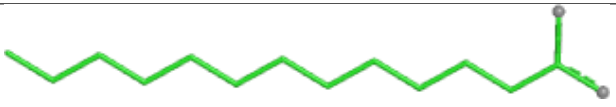
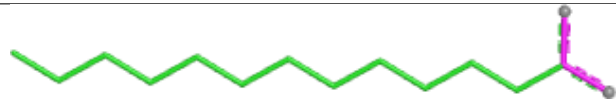
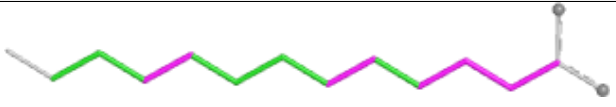
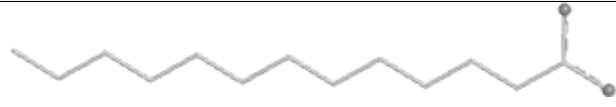
Ligand SQD B 621

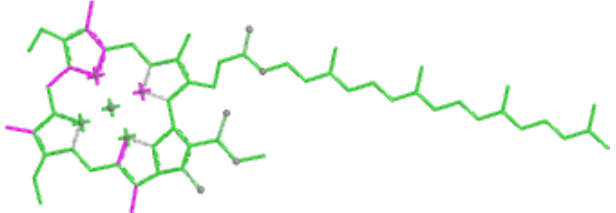
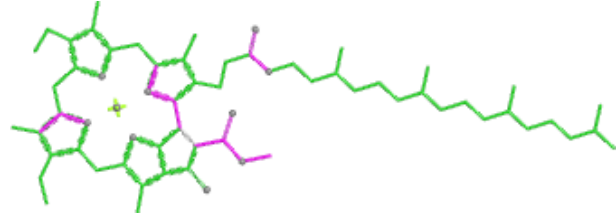
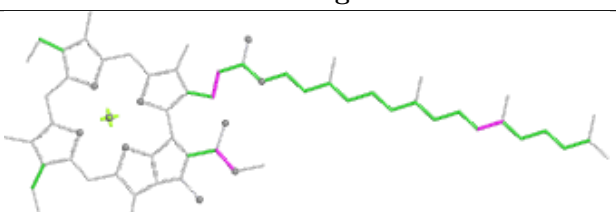
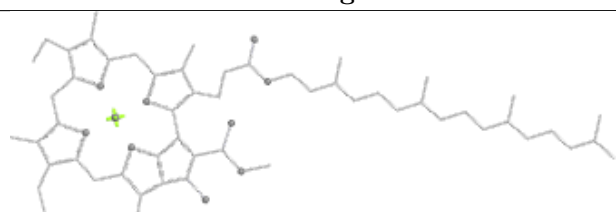


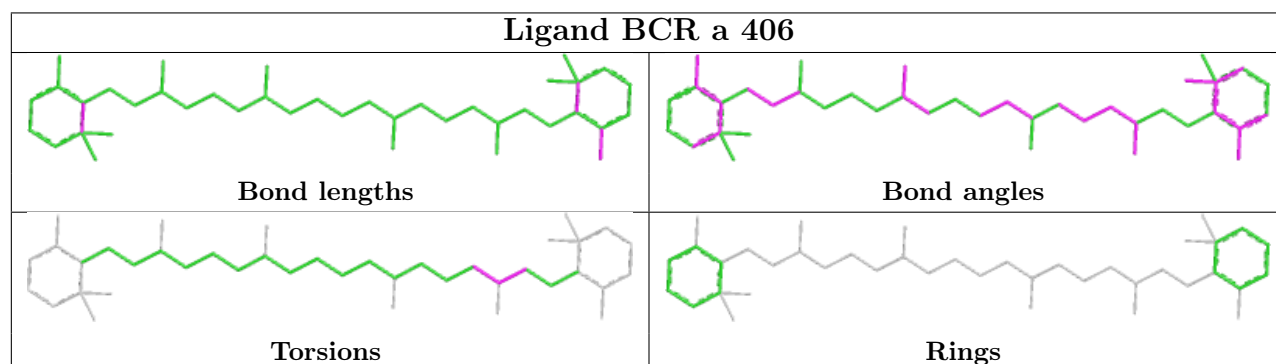
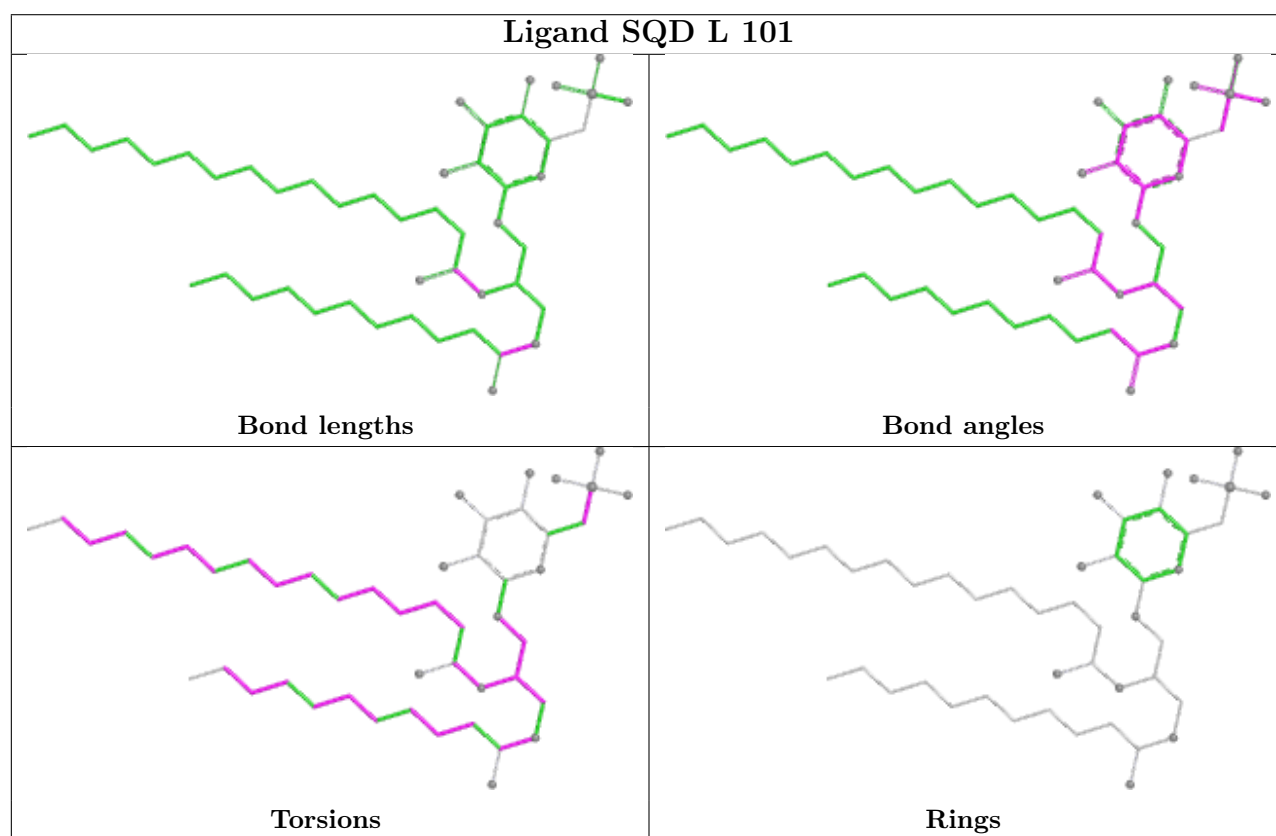
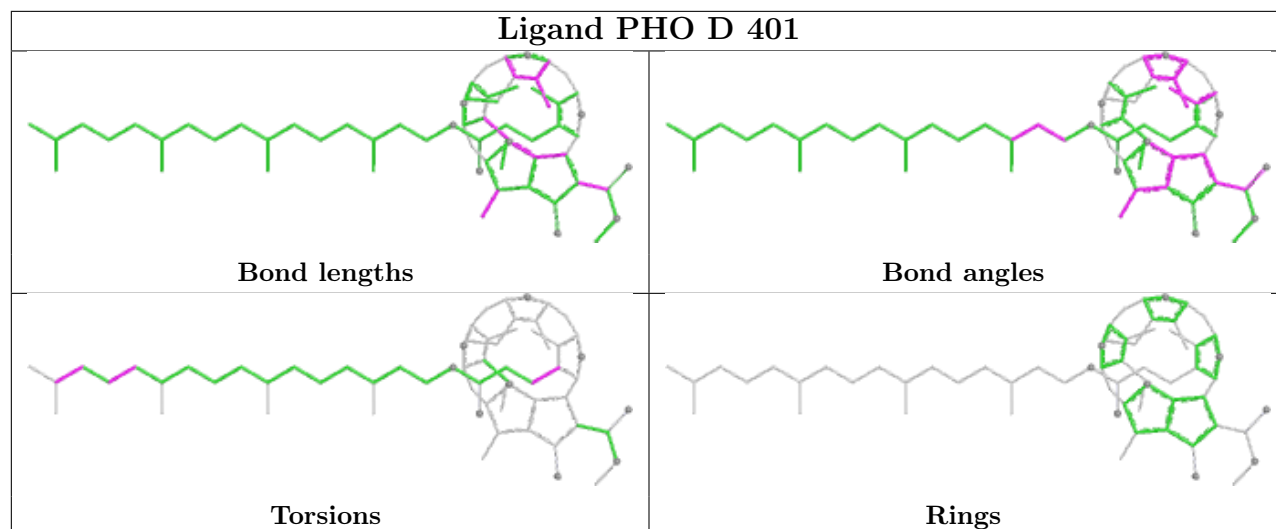
Ligand LHG d 409

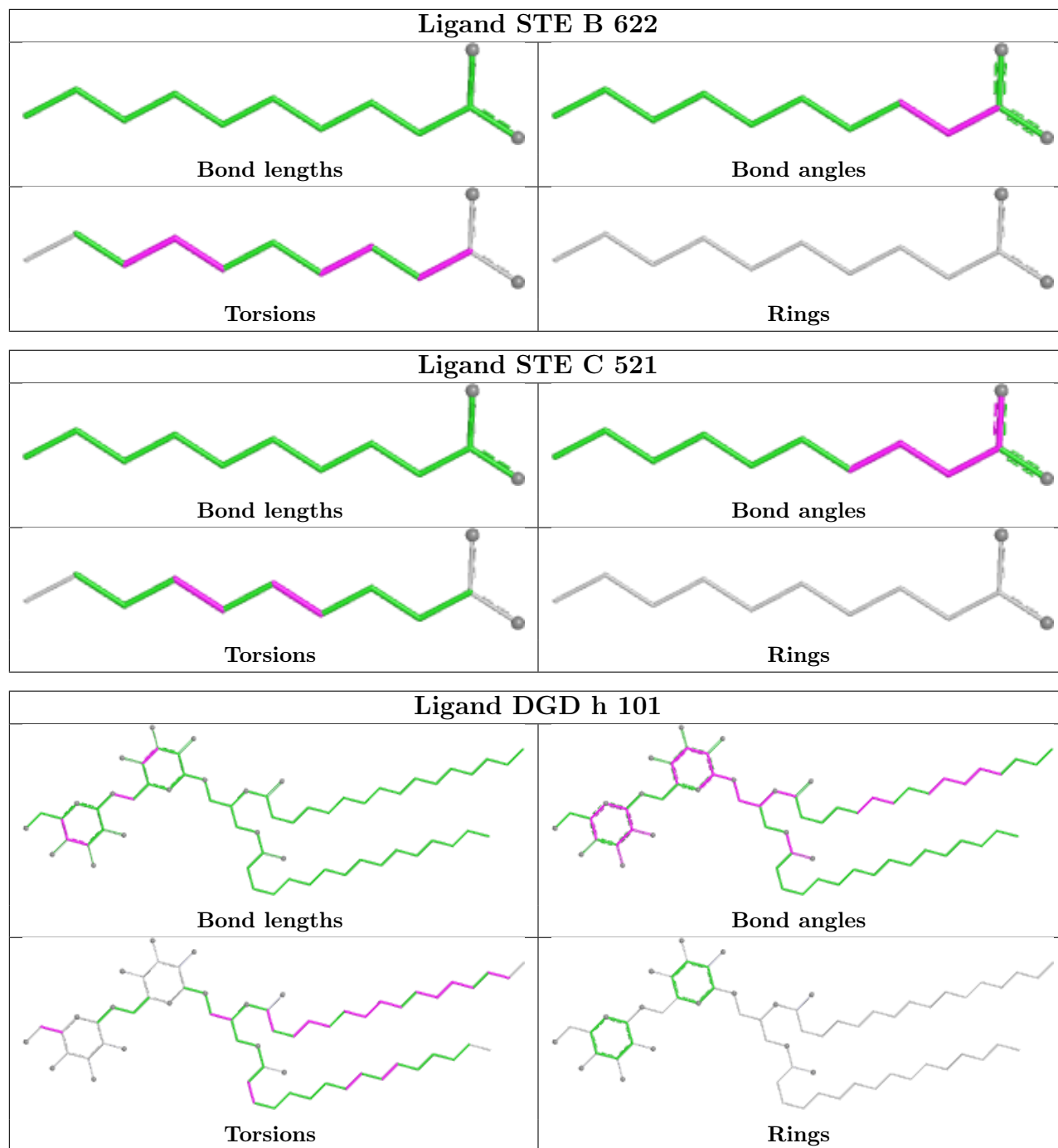


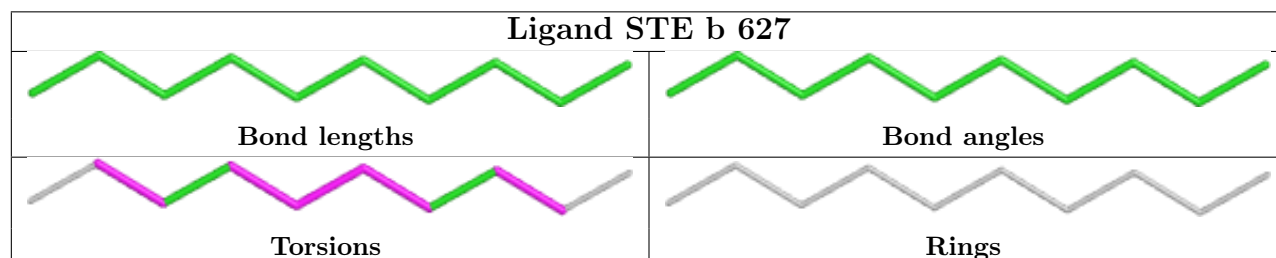
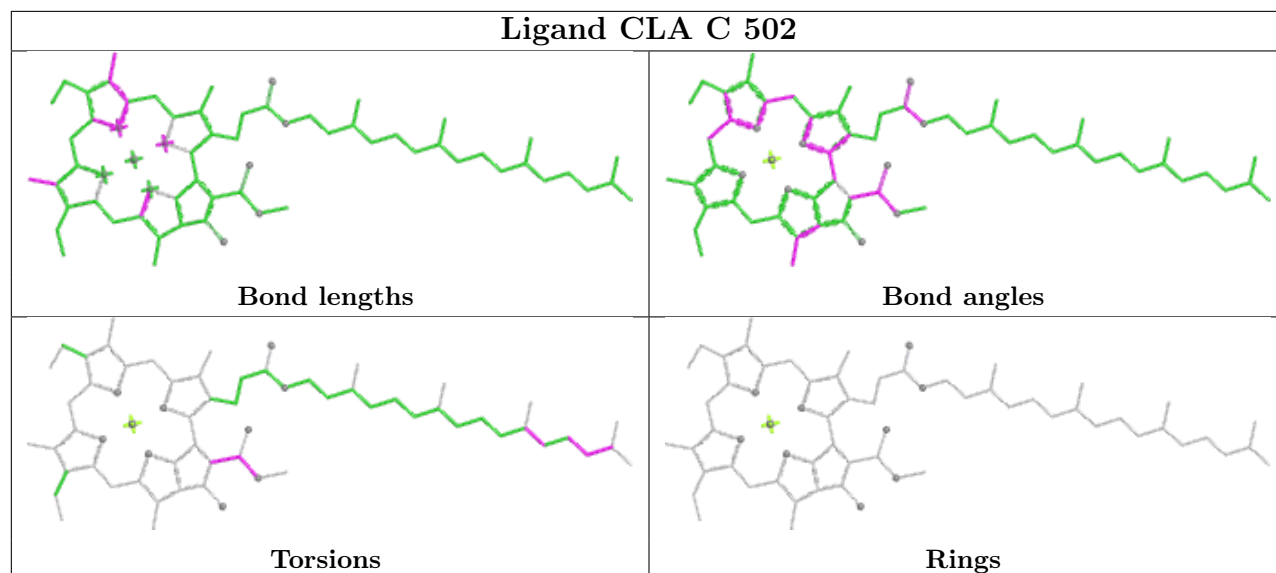
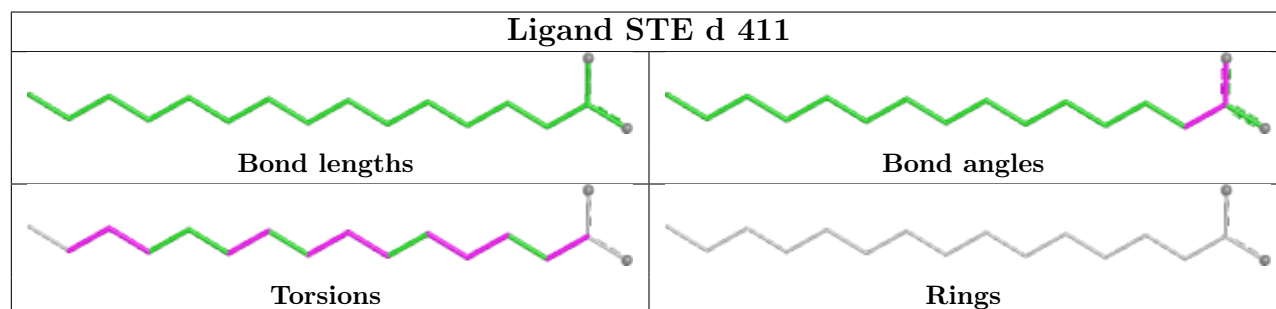
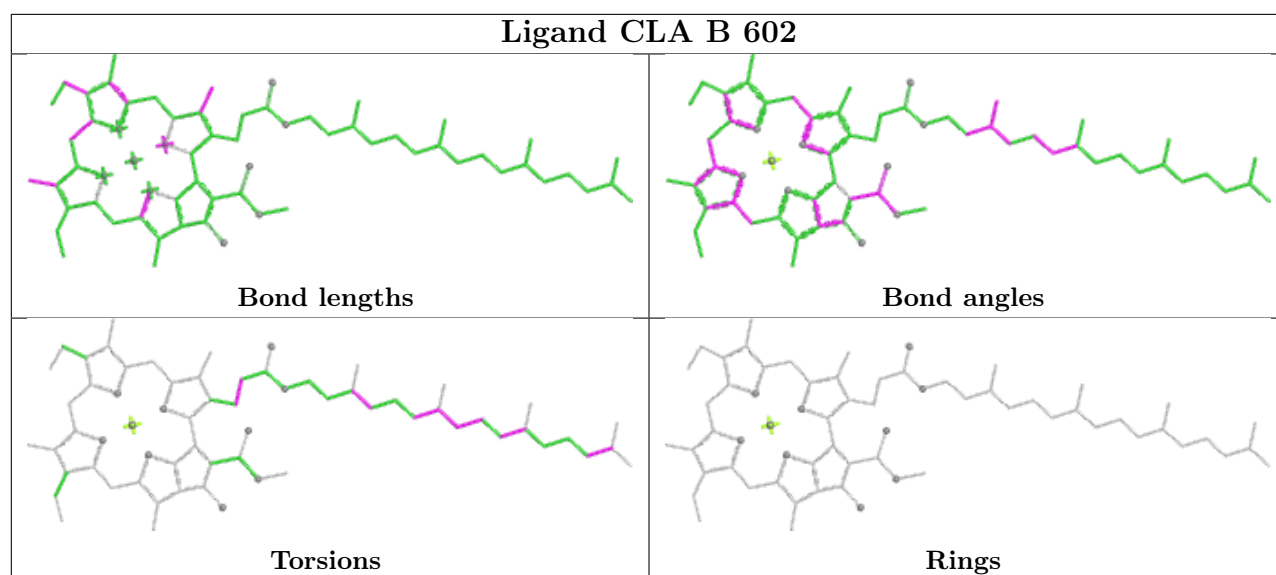
Ligand LMG M 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE M 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

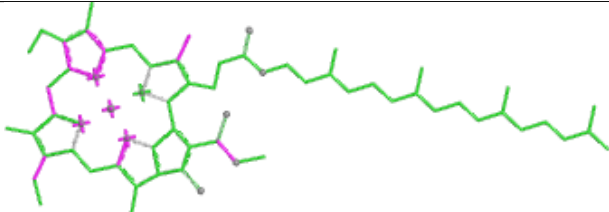
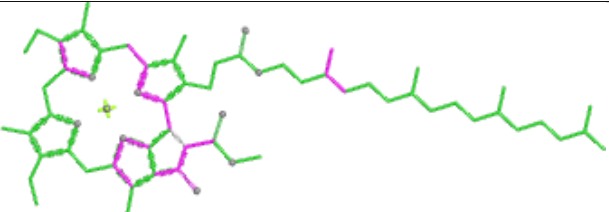
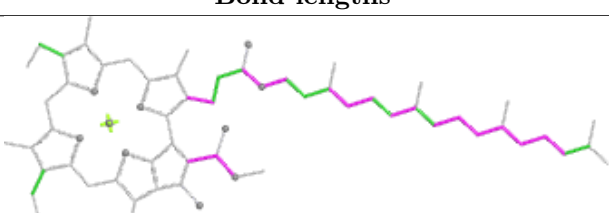
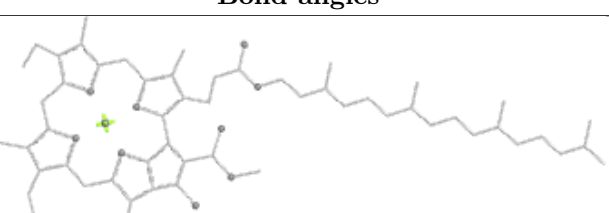
Ligand CLA c 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

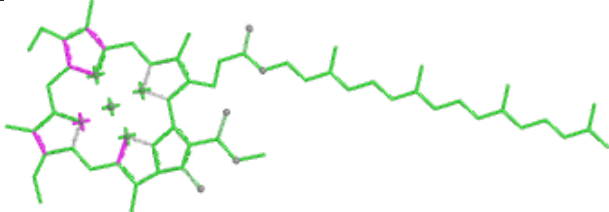
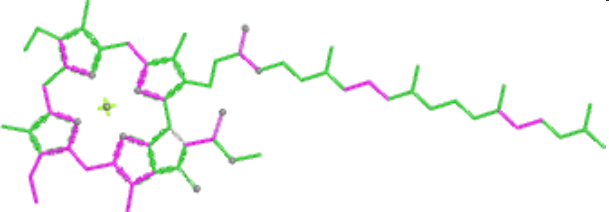
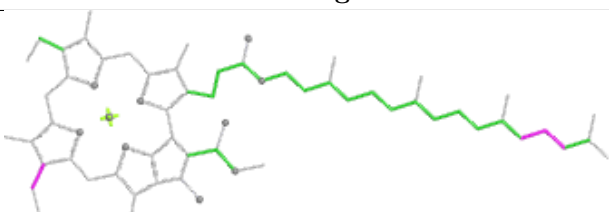
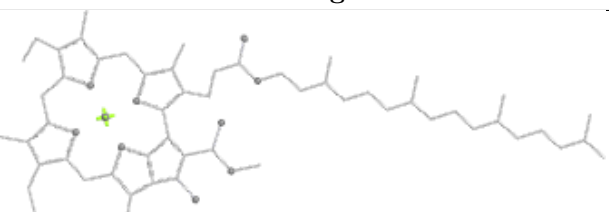




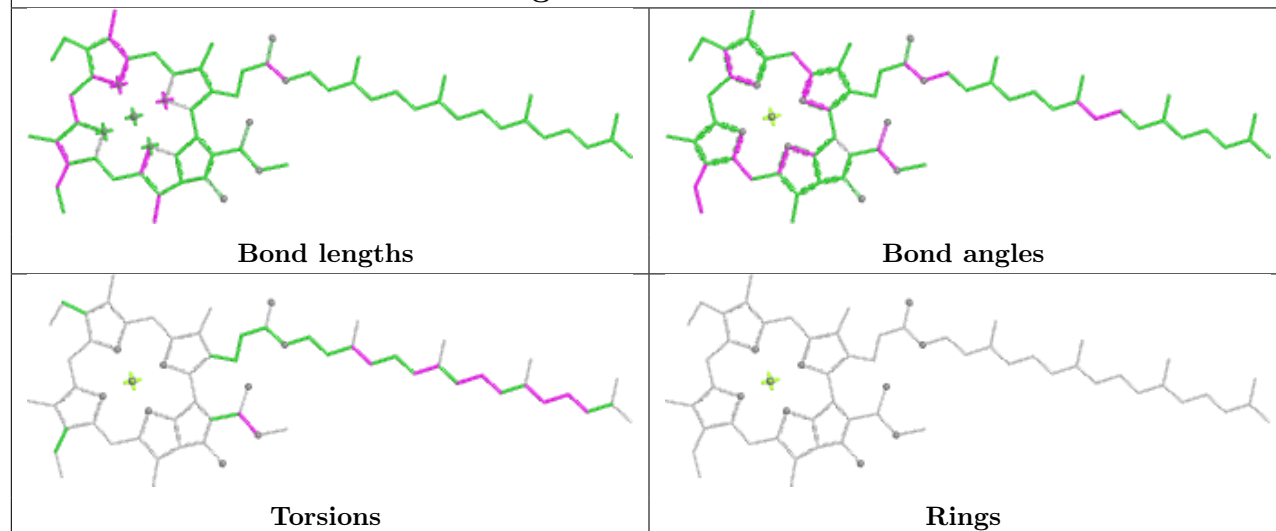


Ligand STE M 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

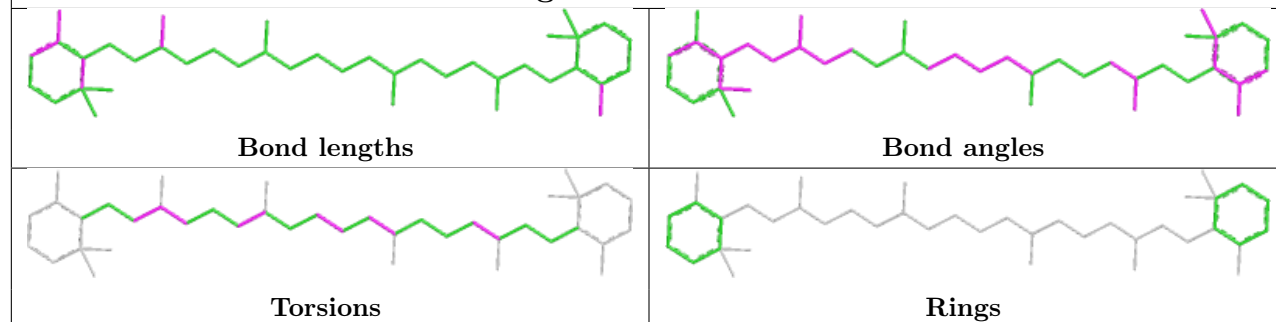
Ligand CLA C 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

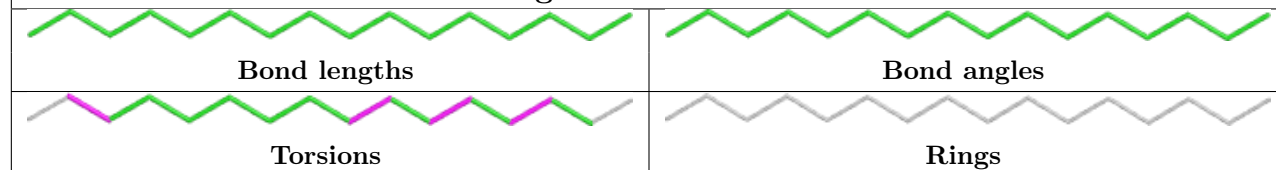
Ligand CLA C 510



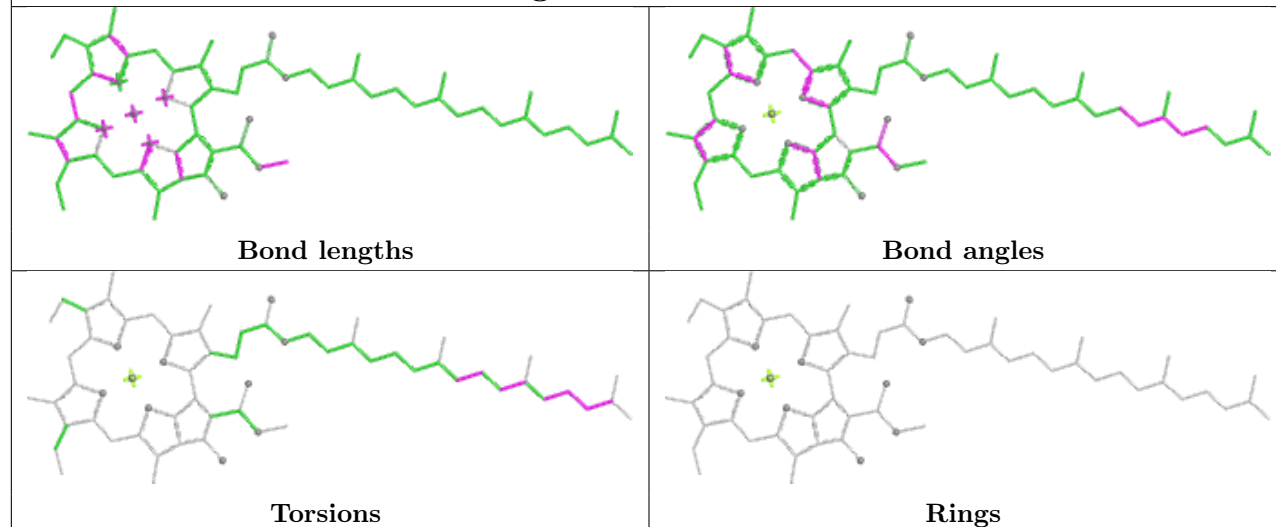
Ligand BCR I 101

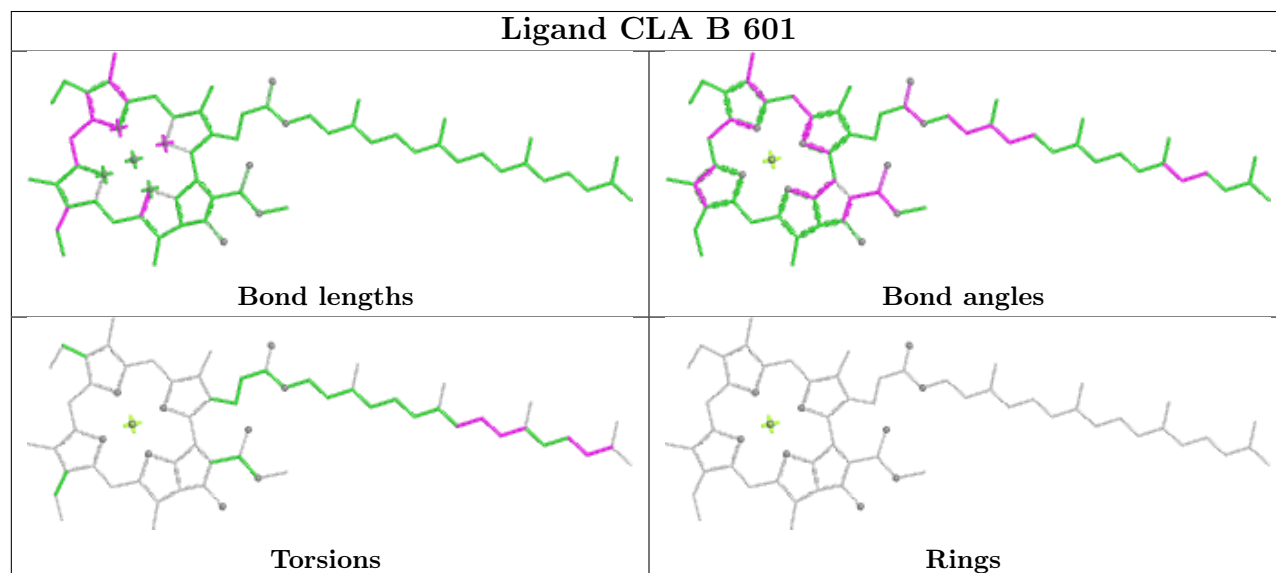
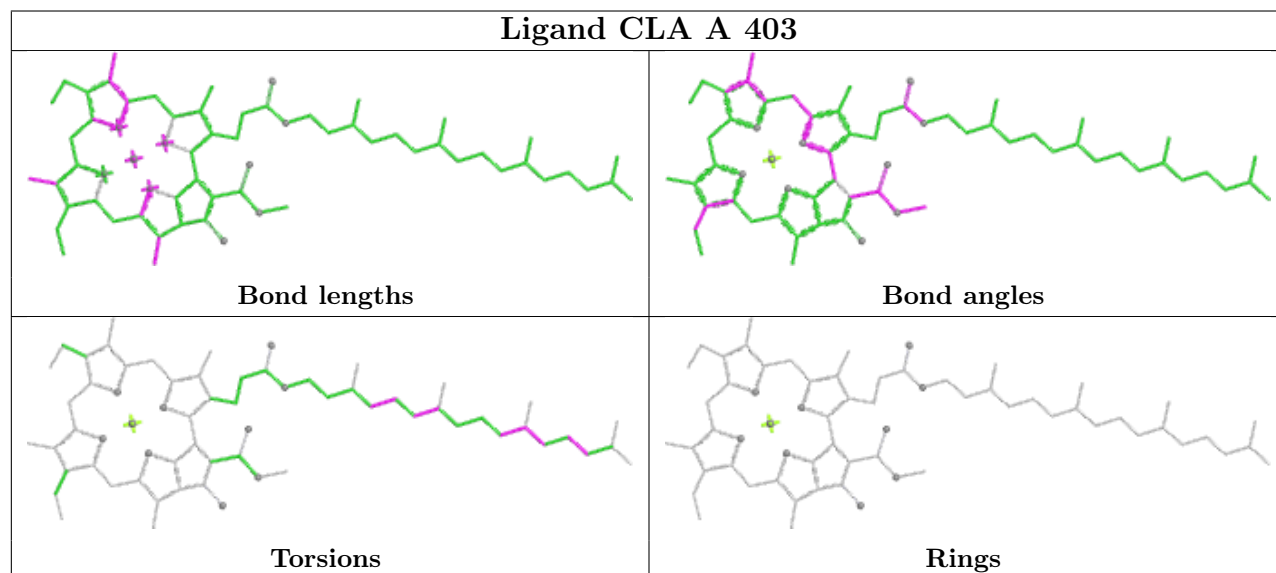
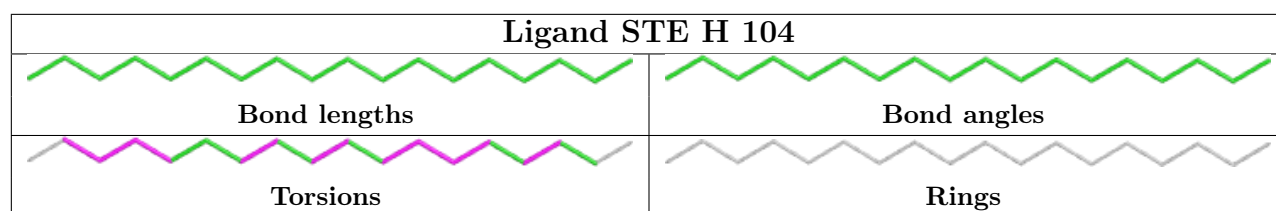


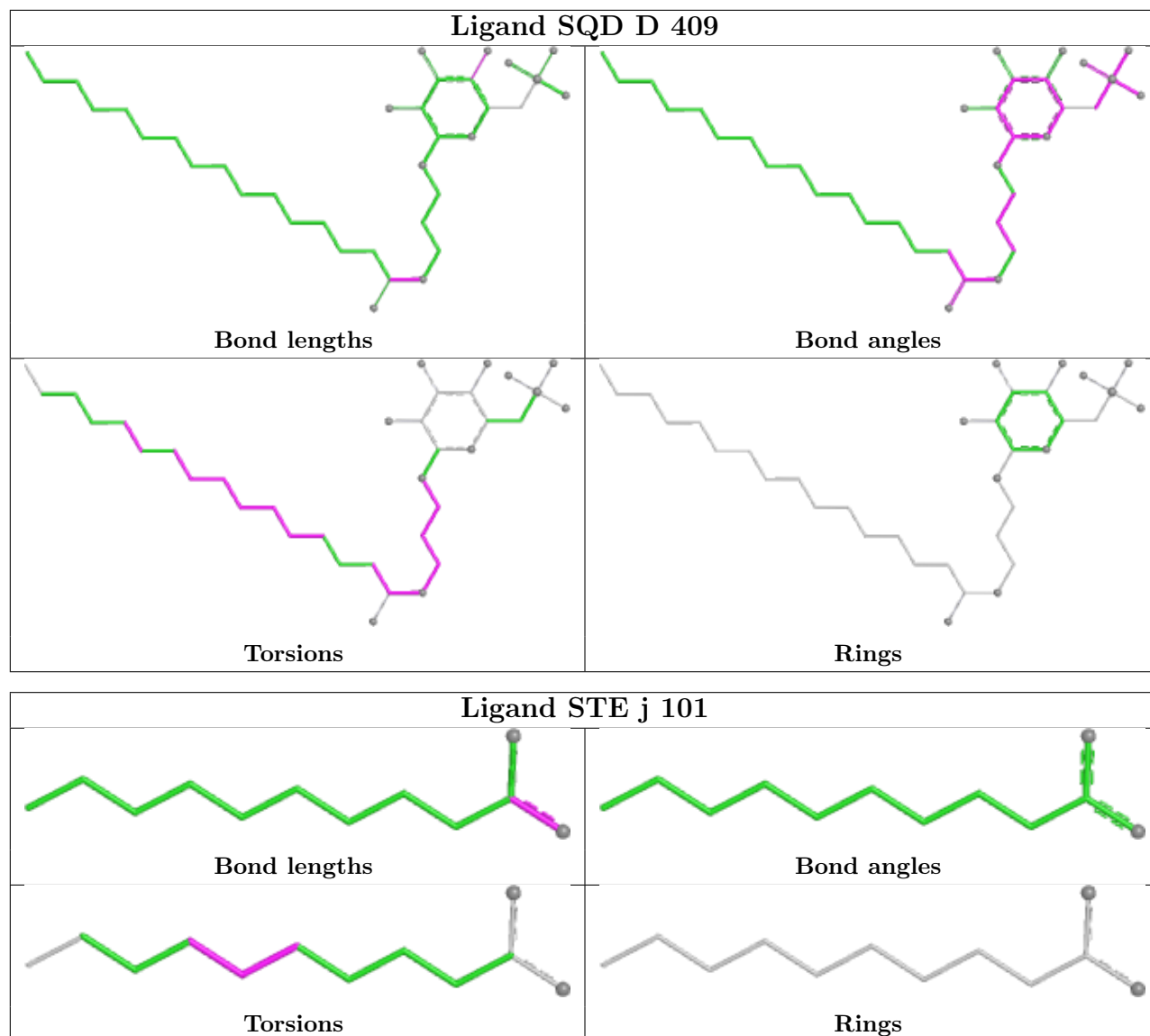
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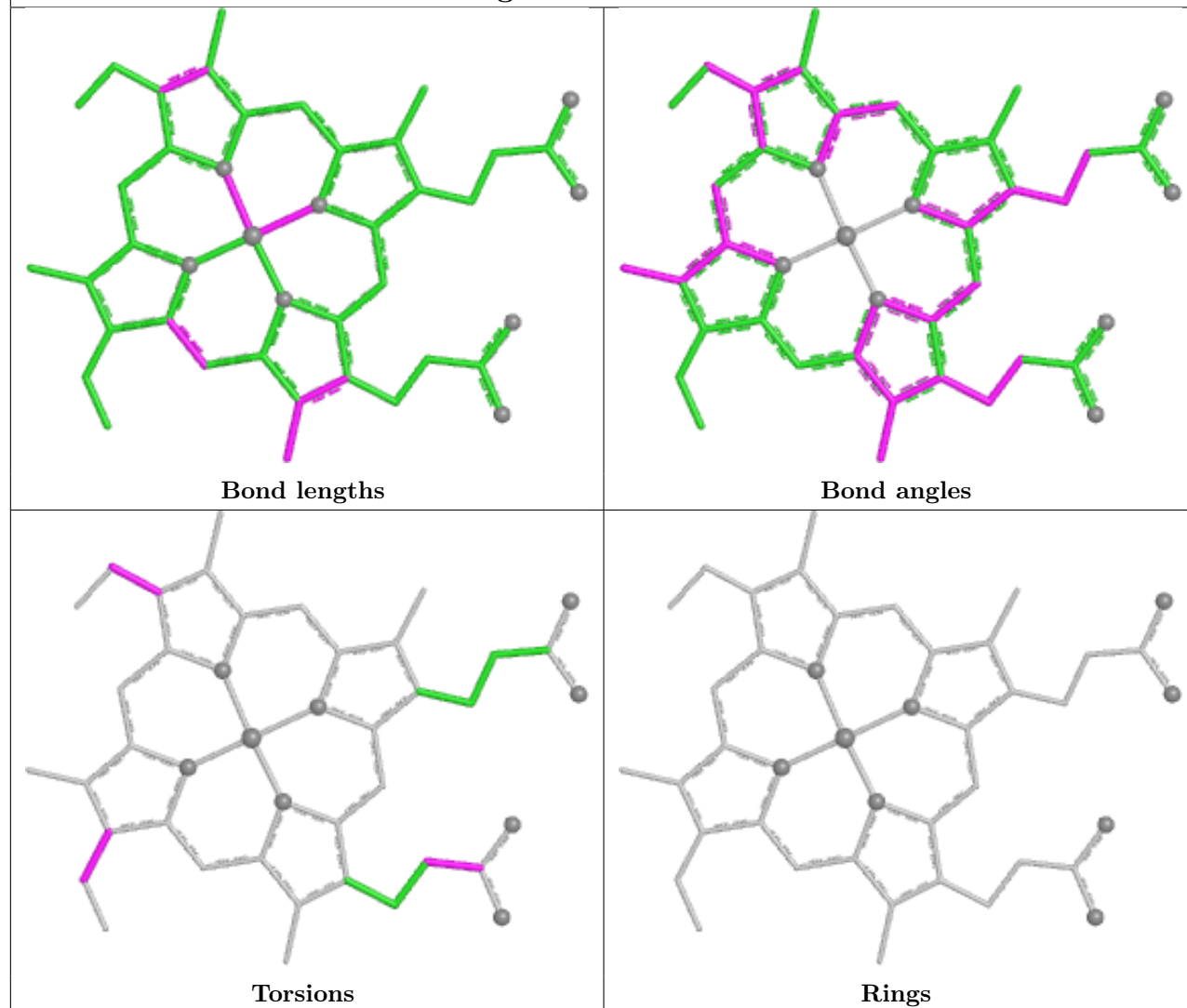
Ligand CLA D 404



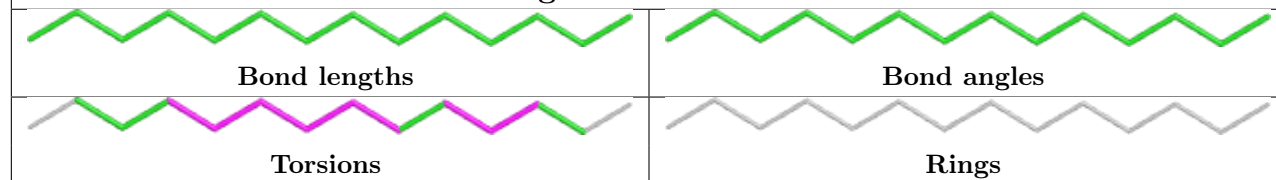


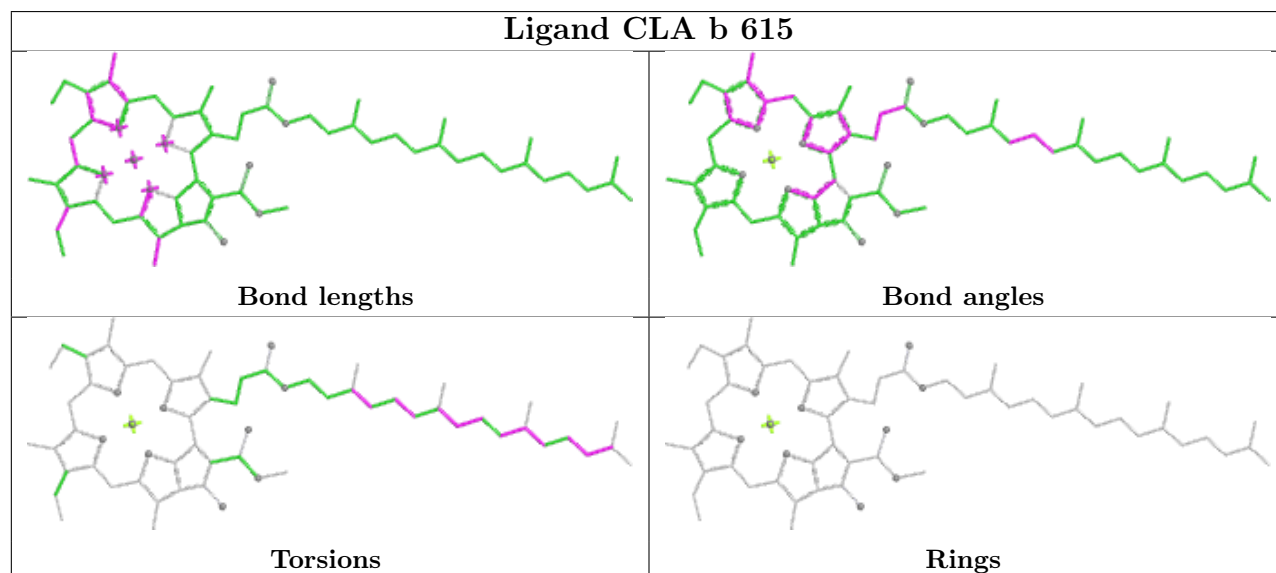
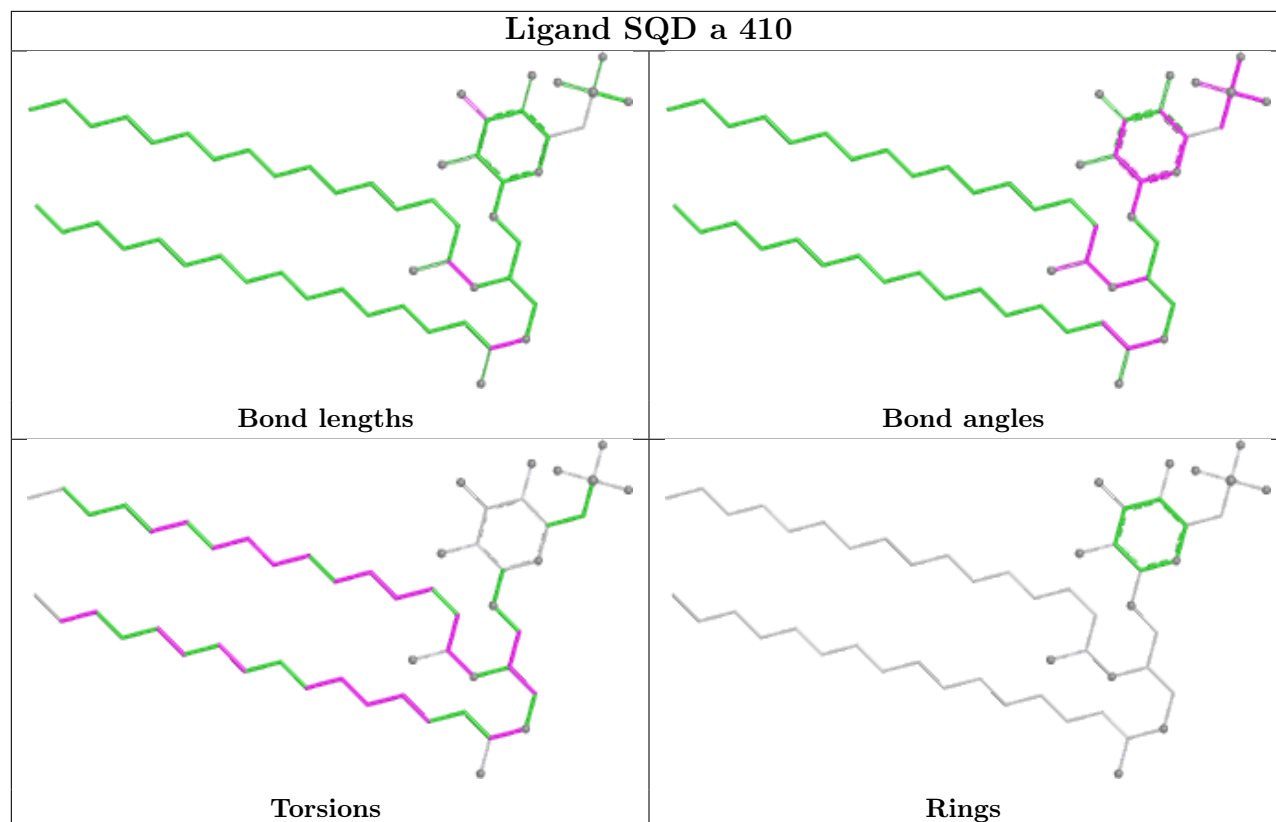


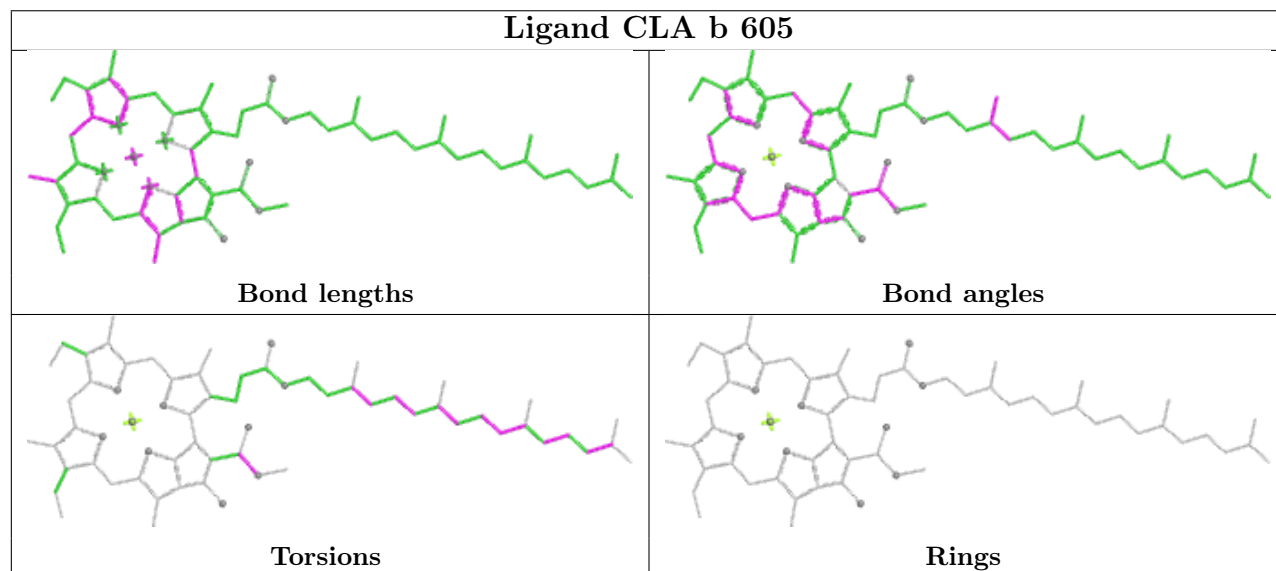
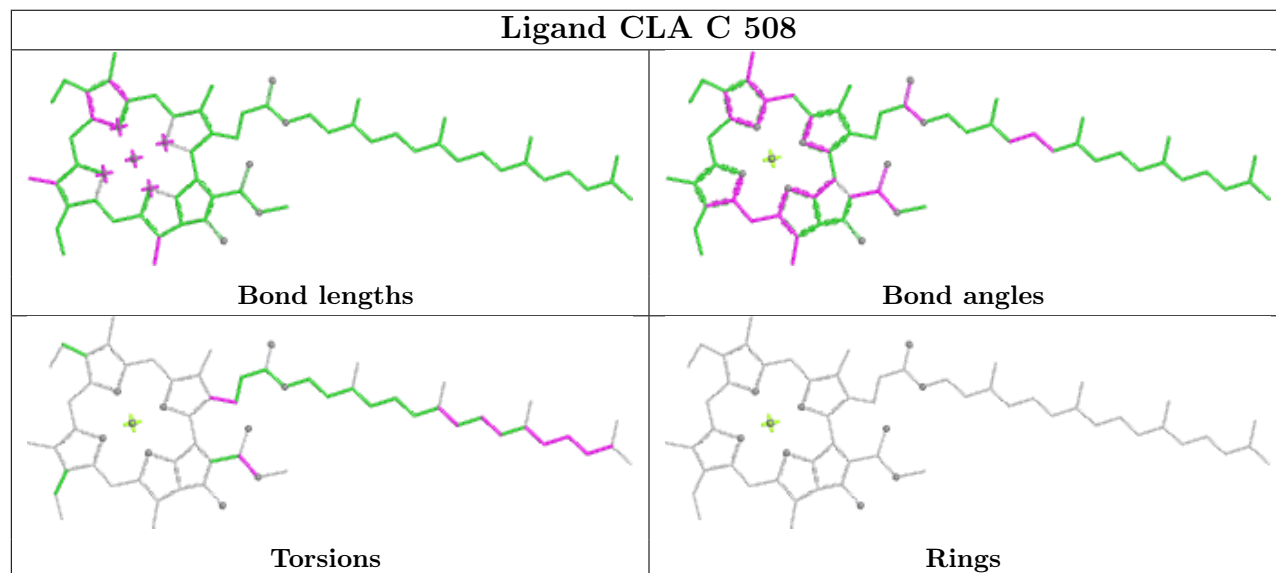
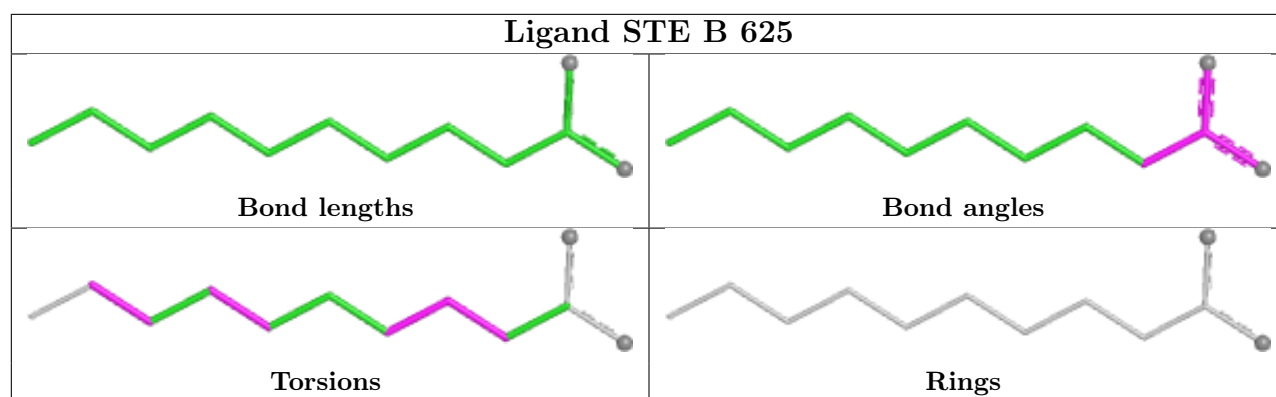
Ligand HEC v 201

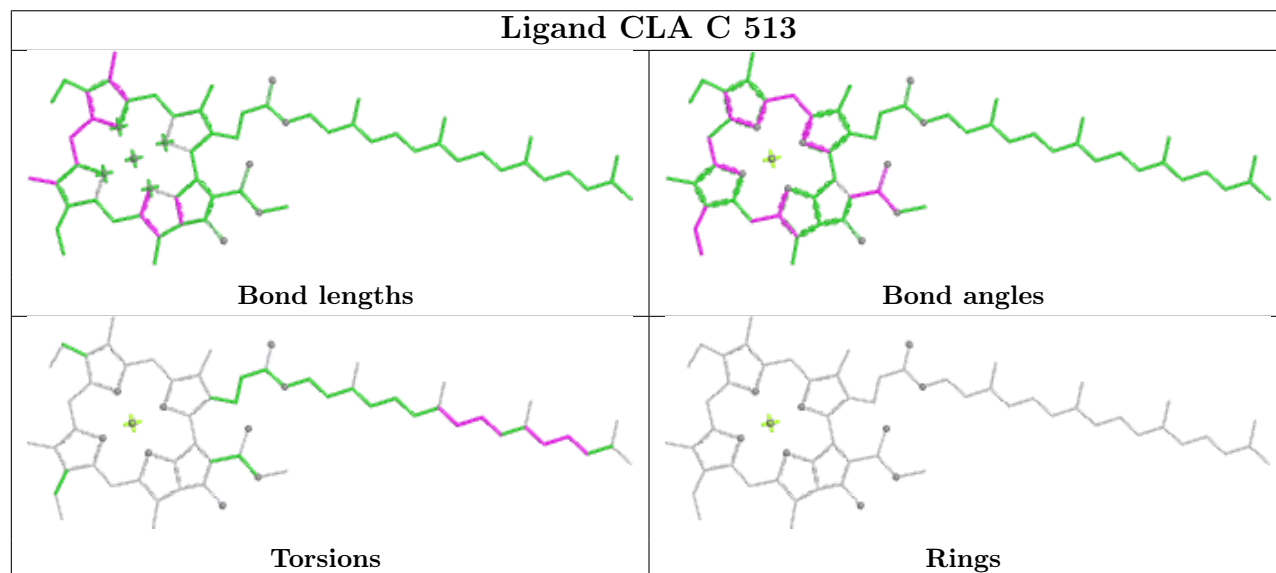
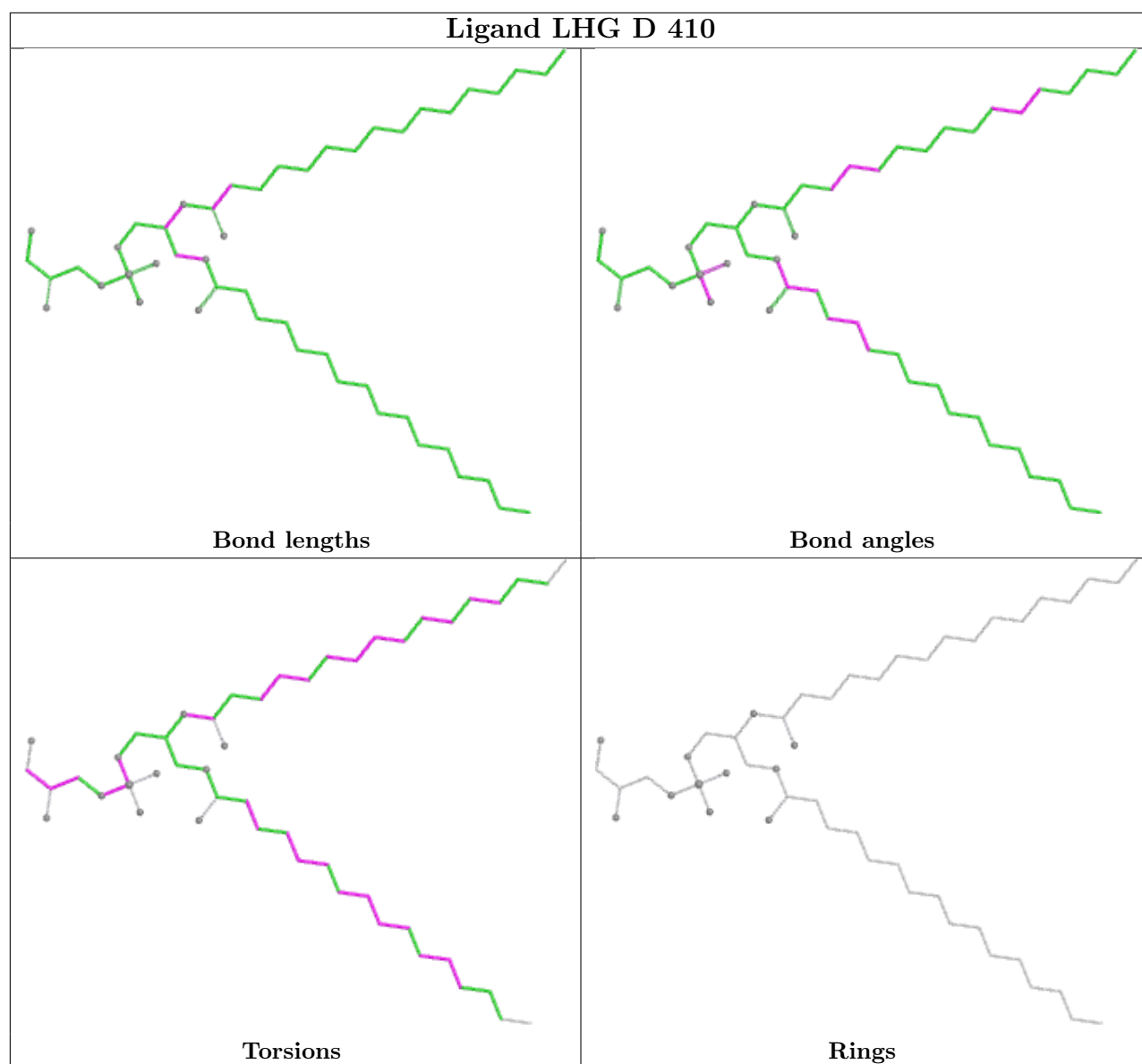


Ligand STE b 628

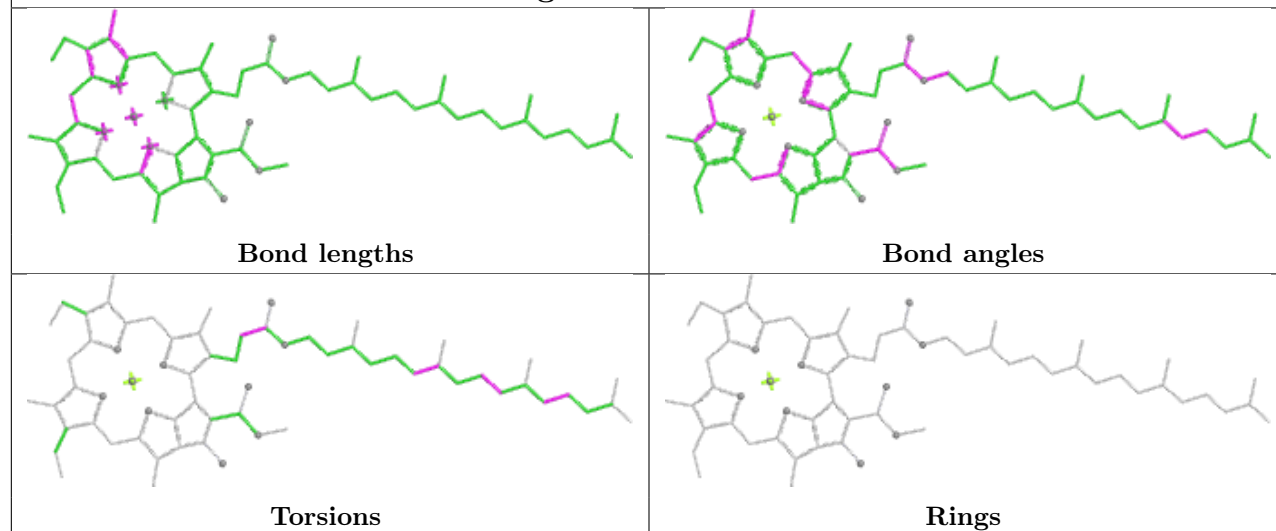




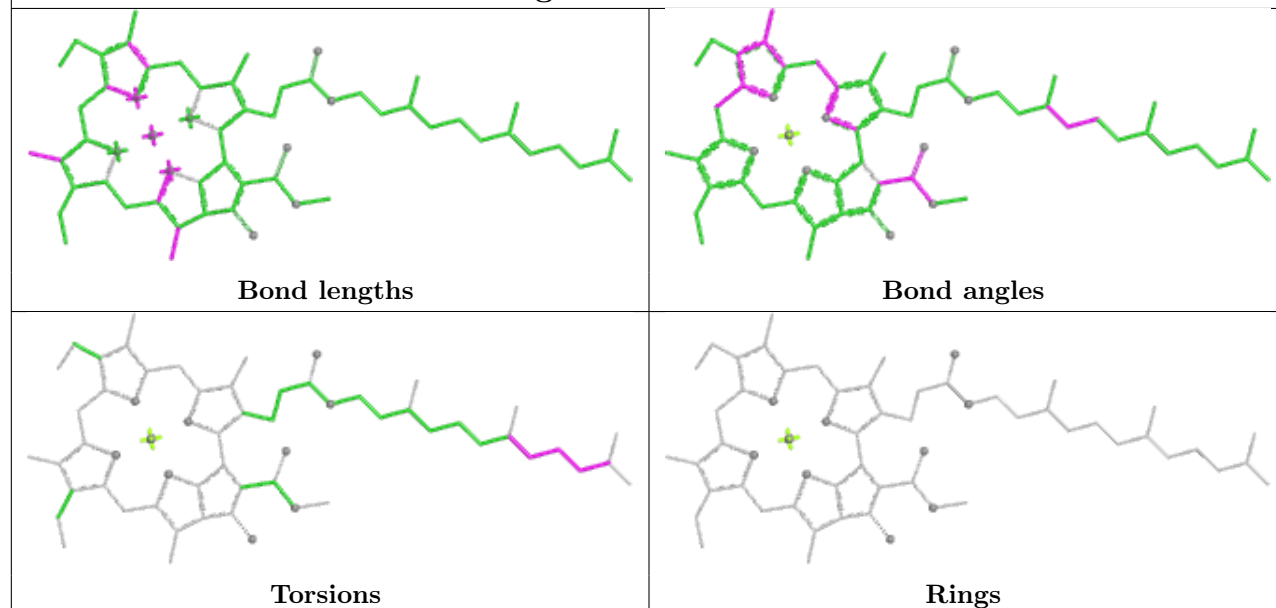


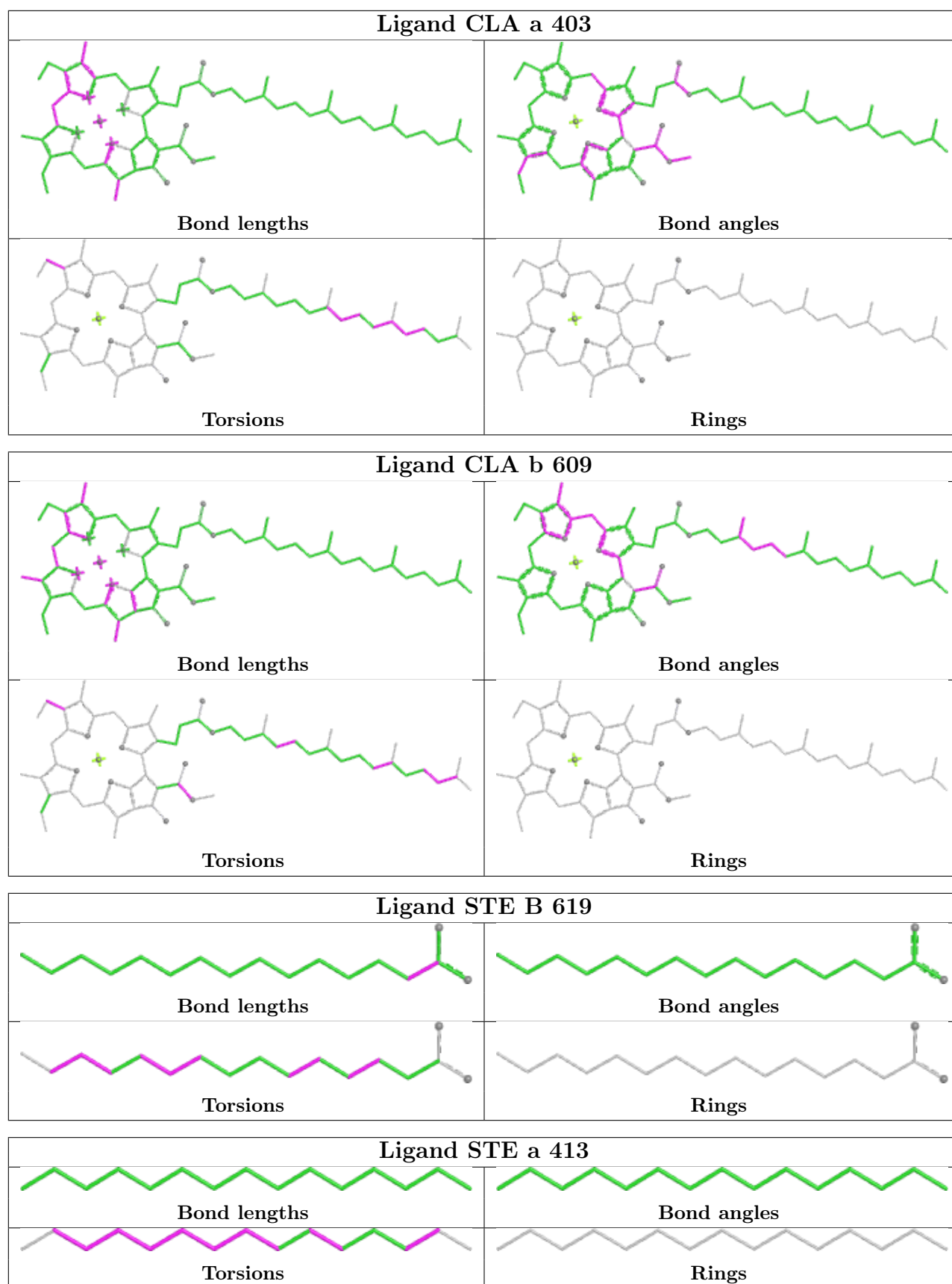


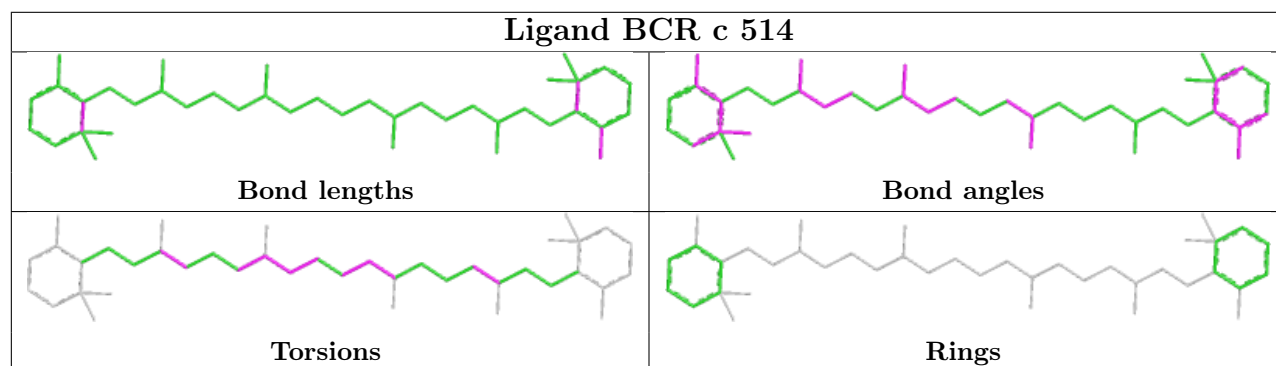
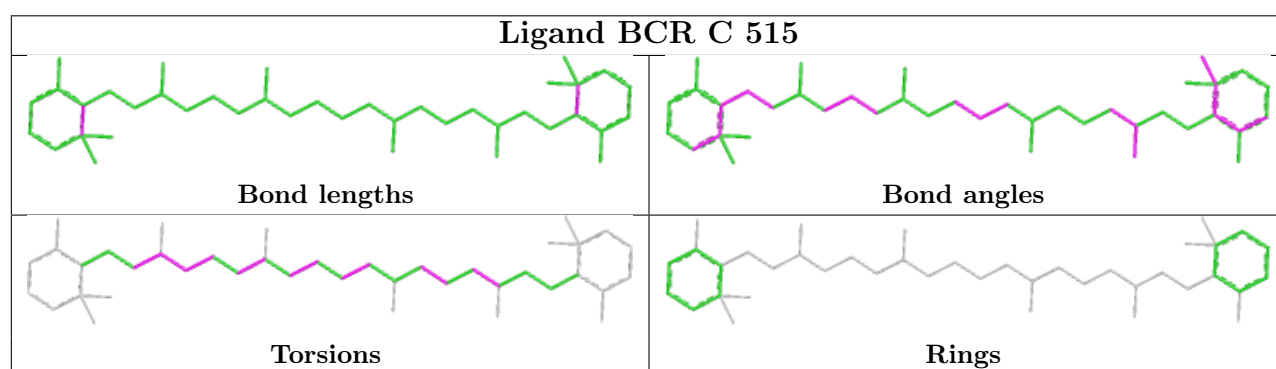
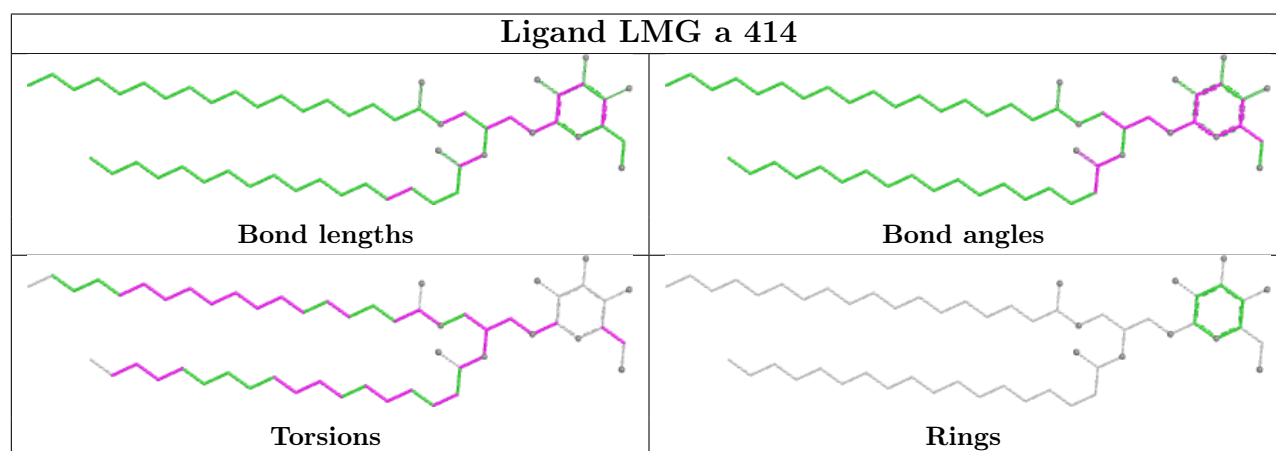
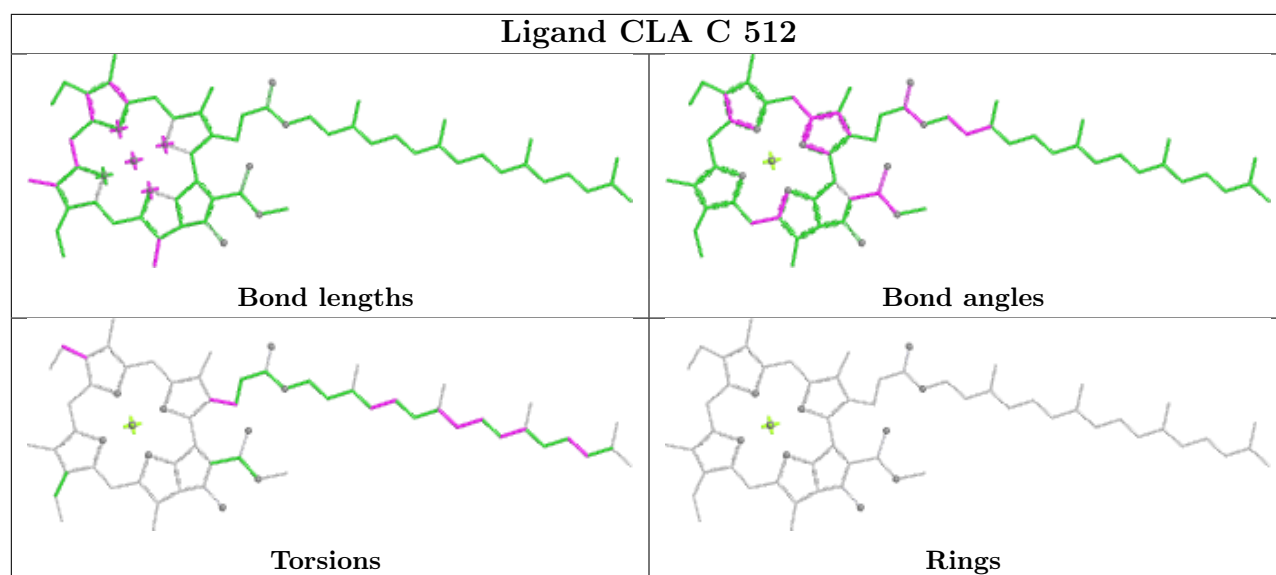
Ligand CLA c 509

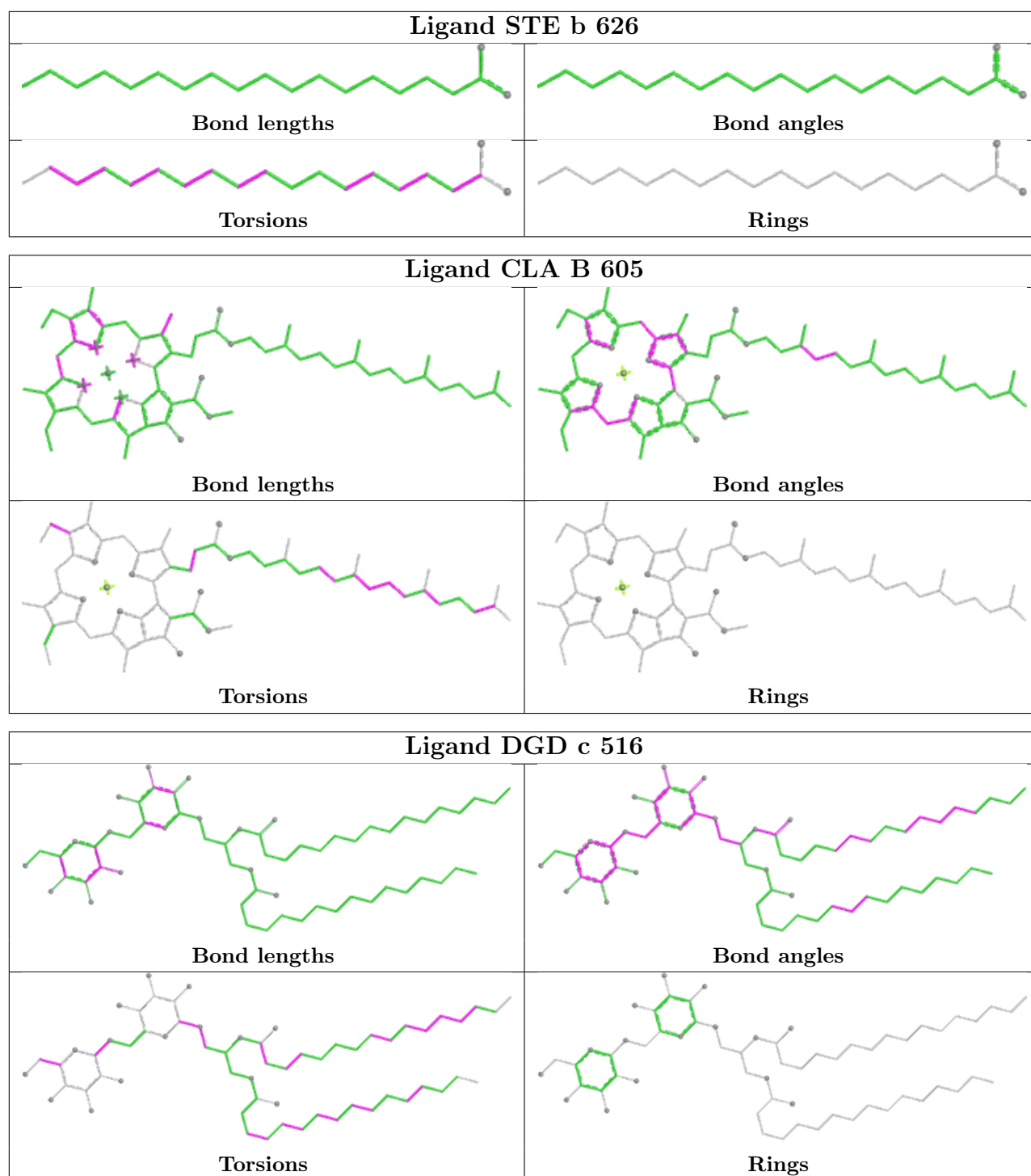


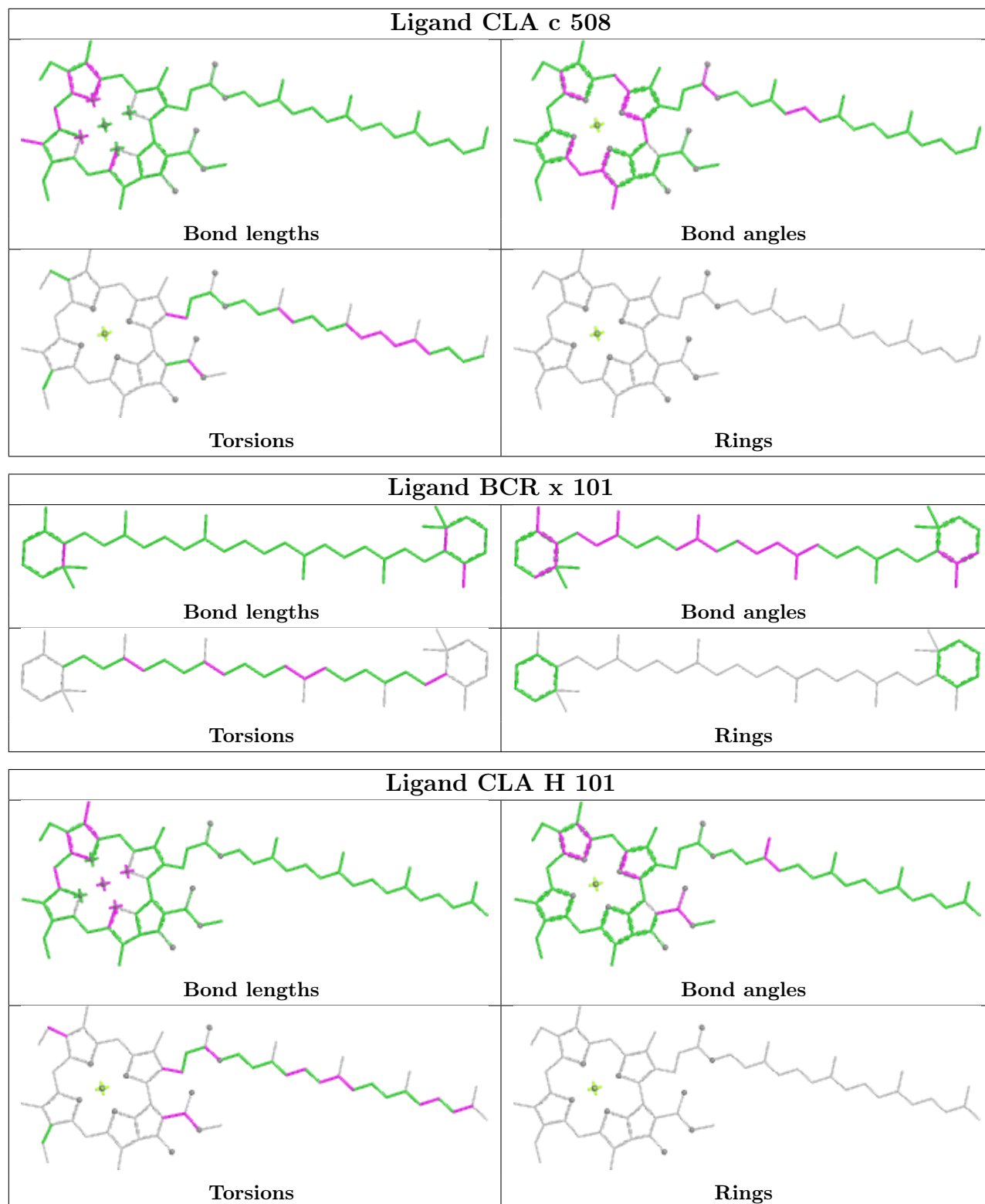
Ligand CLA b 616

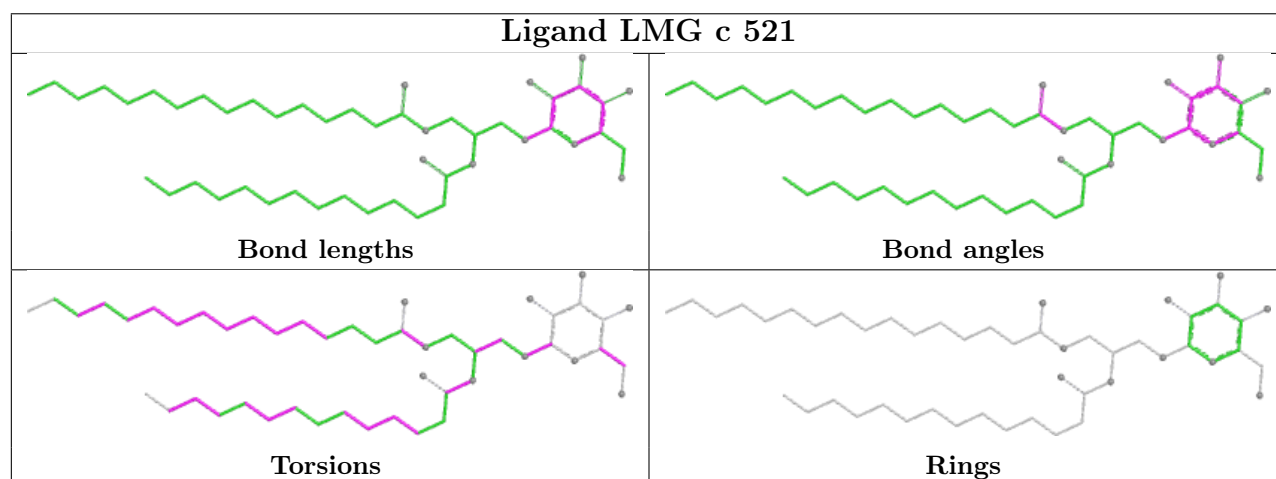
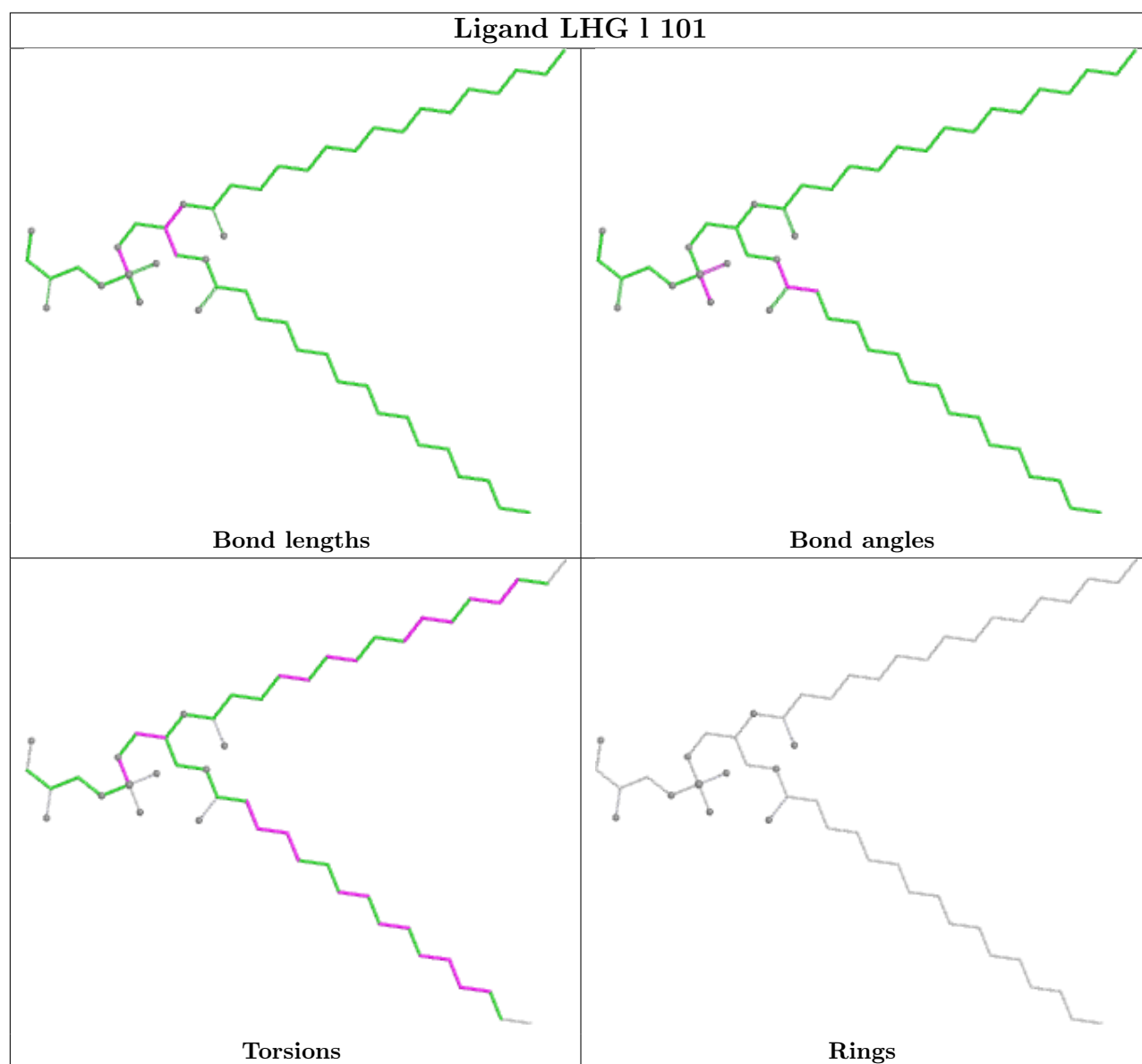


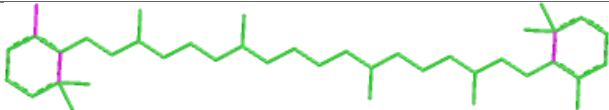
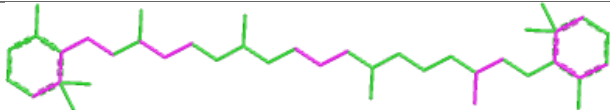
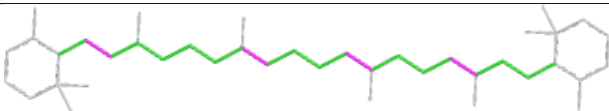
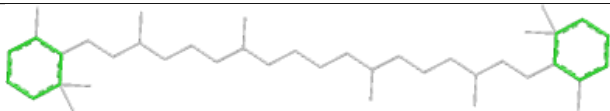


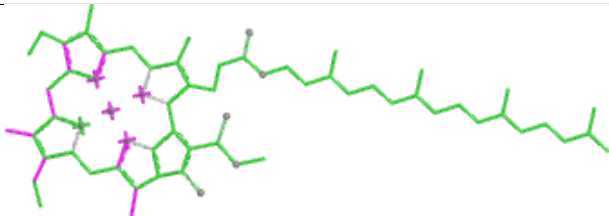
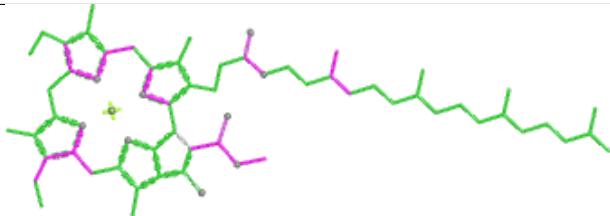
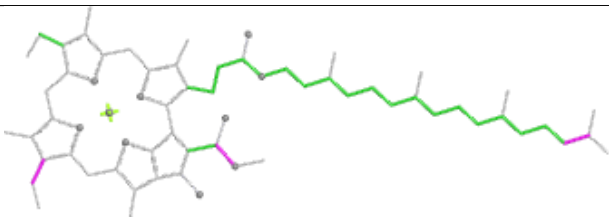
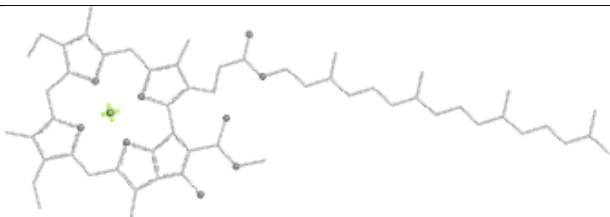


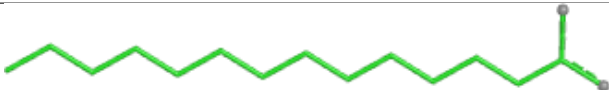
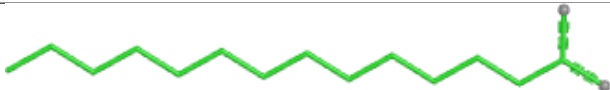
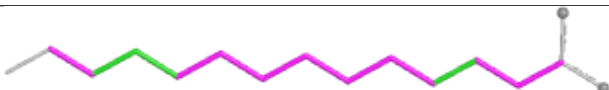
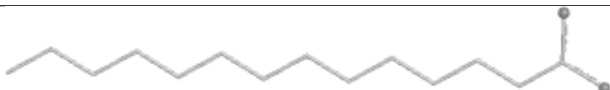




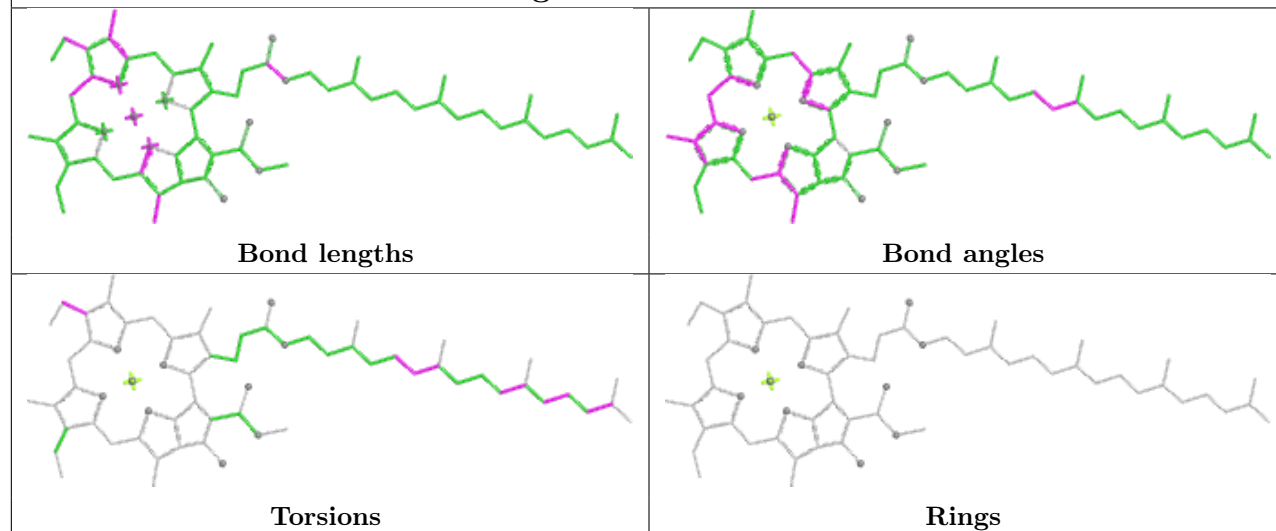


Ligand BCR B 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

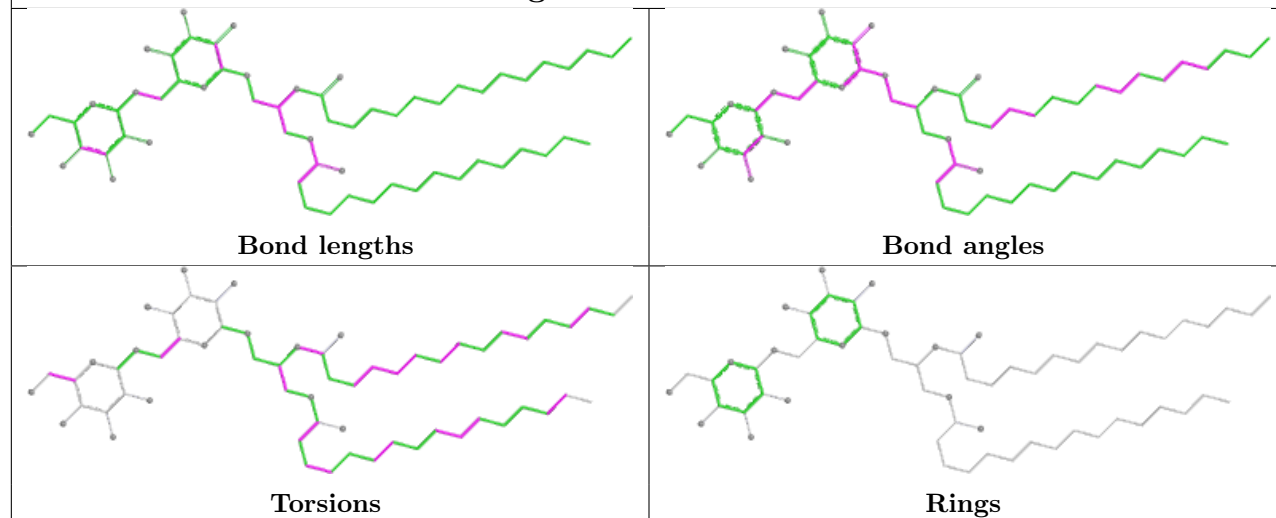
Ligand CLA C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE b 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

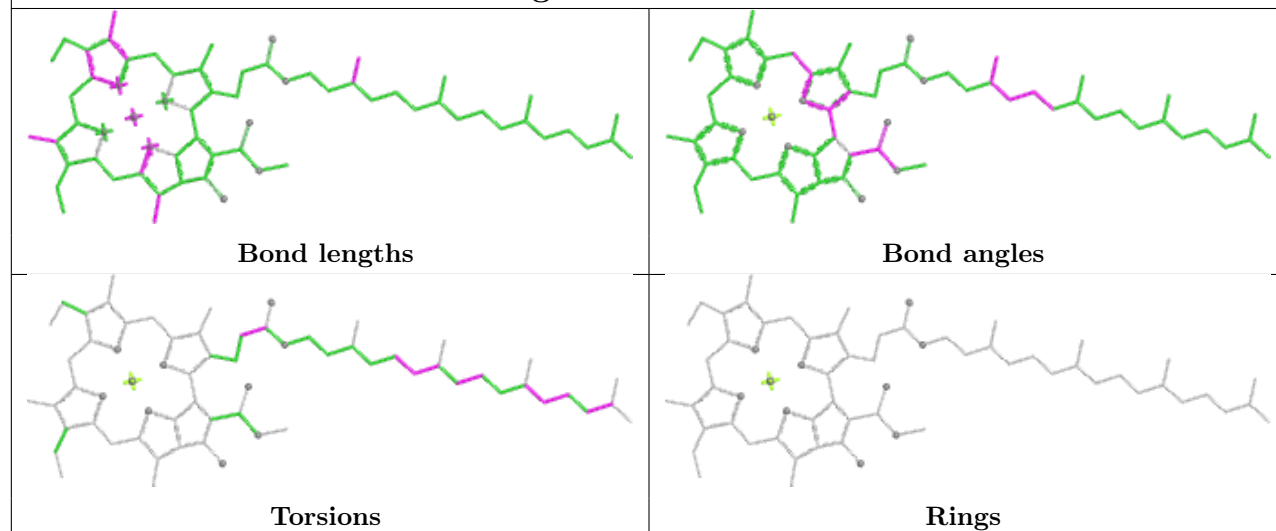
Ligand CLA B 614



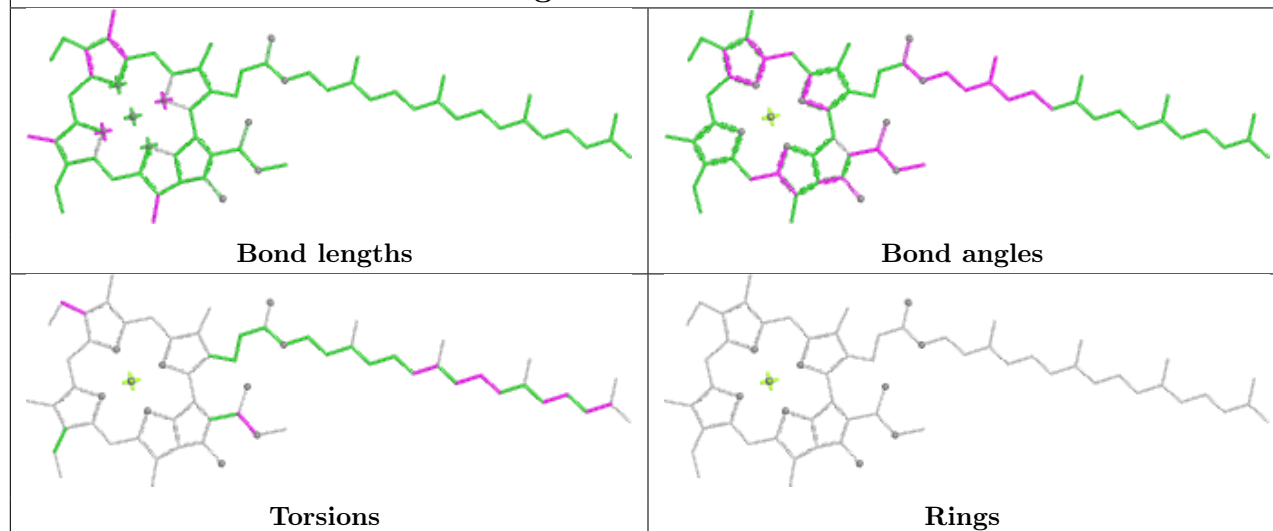
Ligand DGD C 516



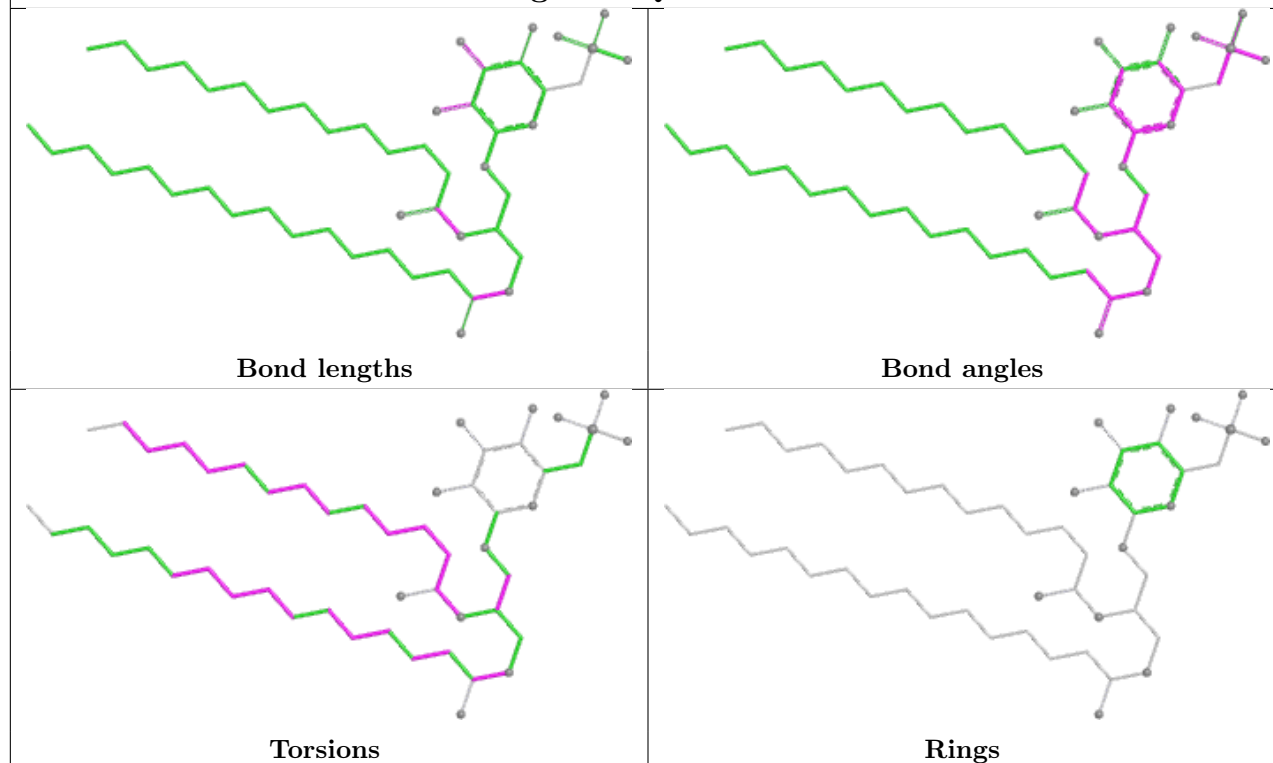
Ligand CLA B 612



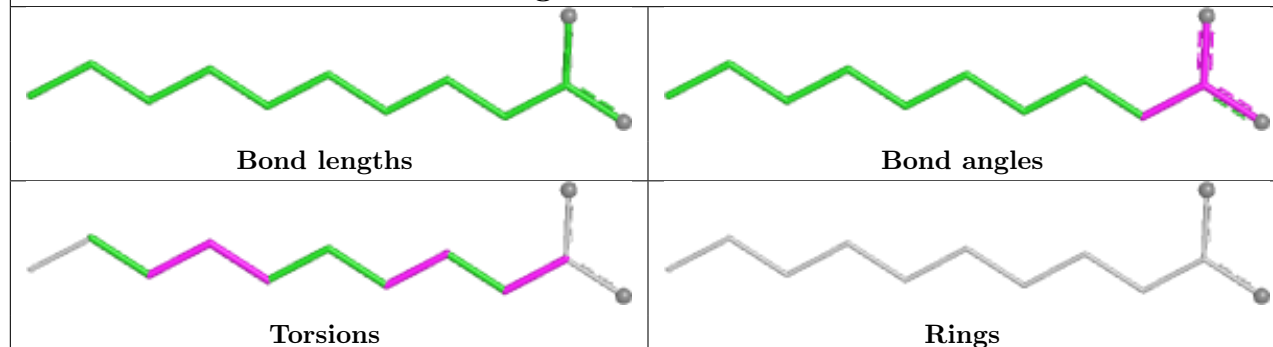
Ligand CLA b 603

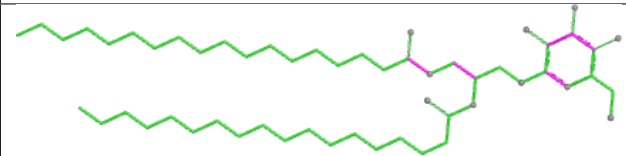
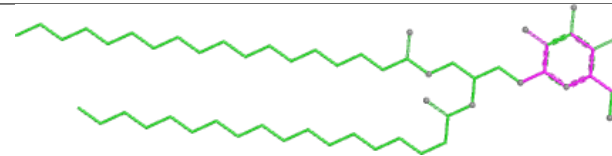
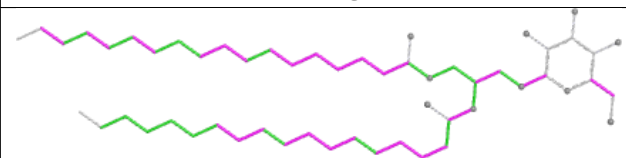
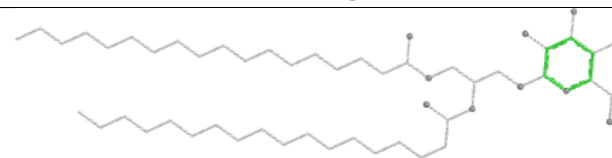
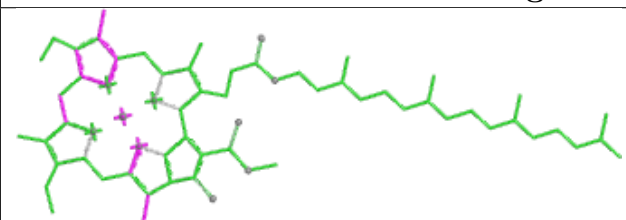
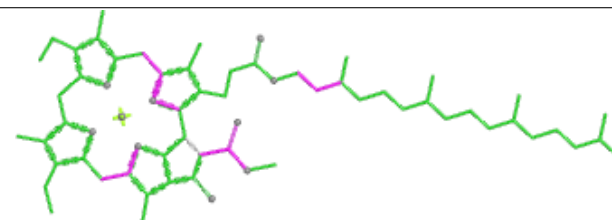
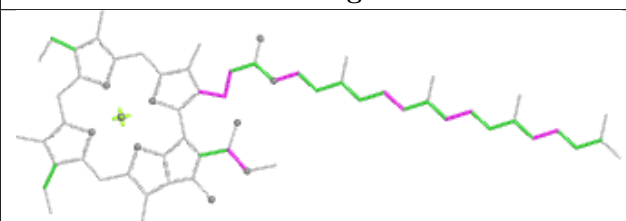
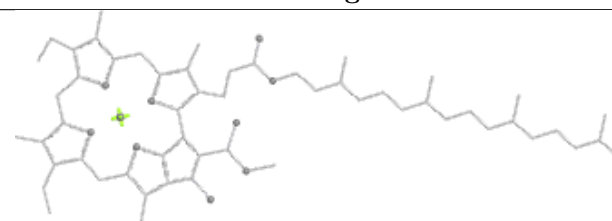
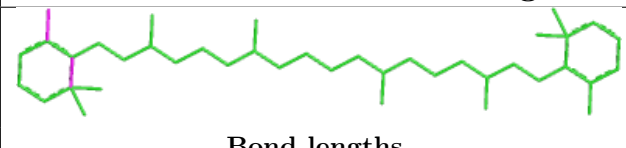
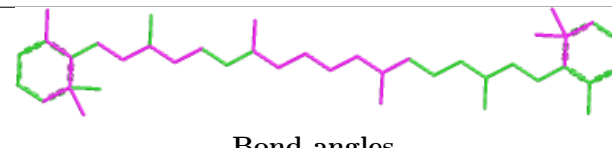
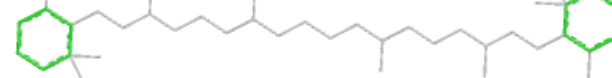


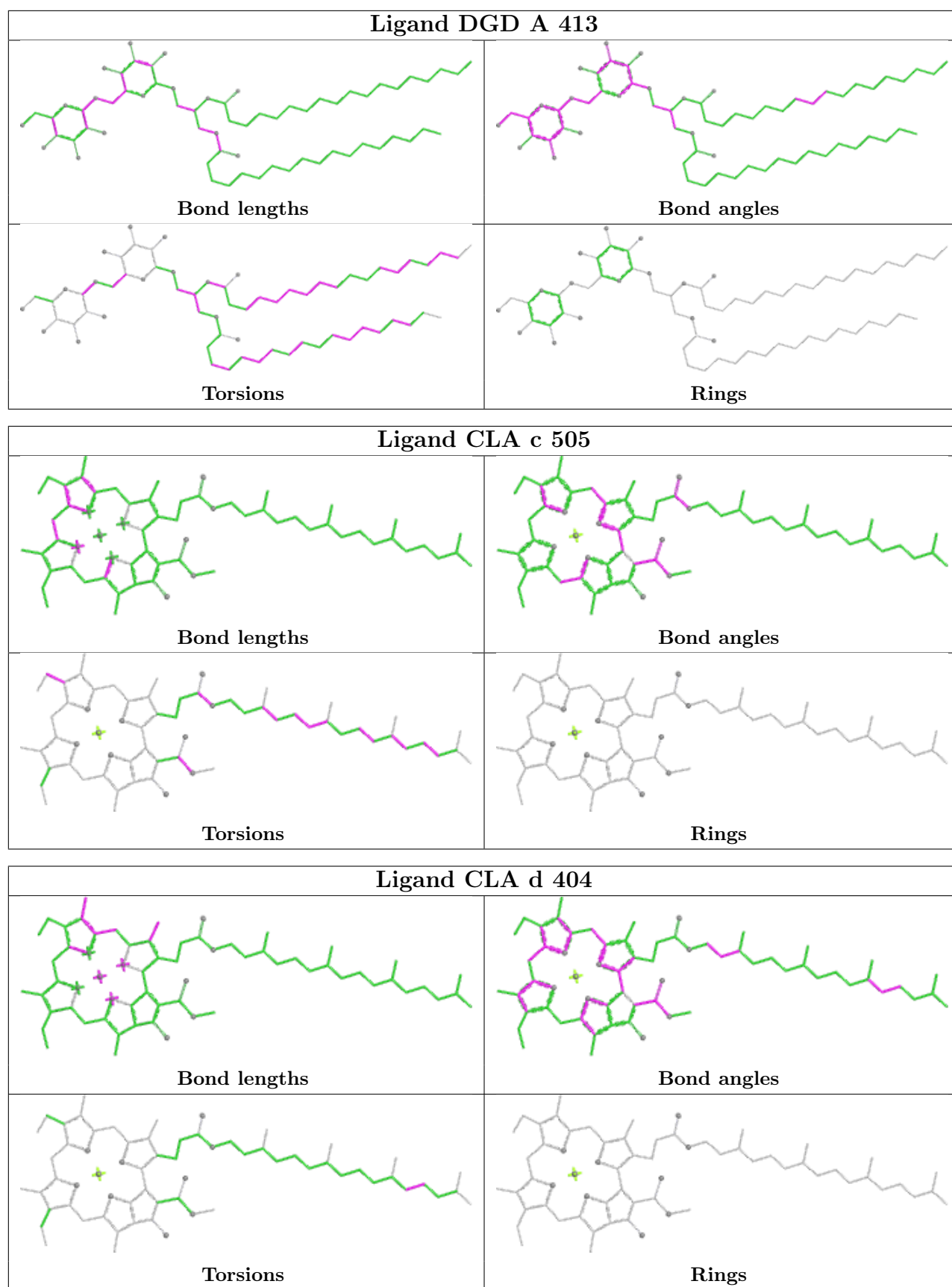
Ligand SQD A 410

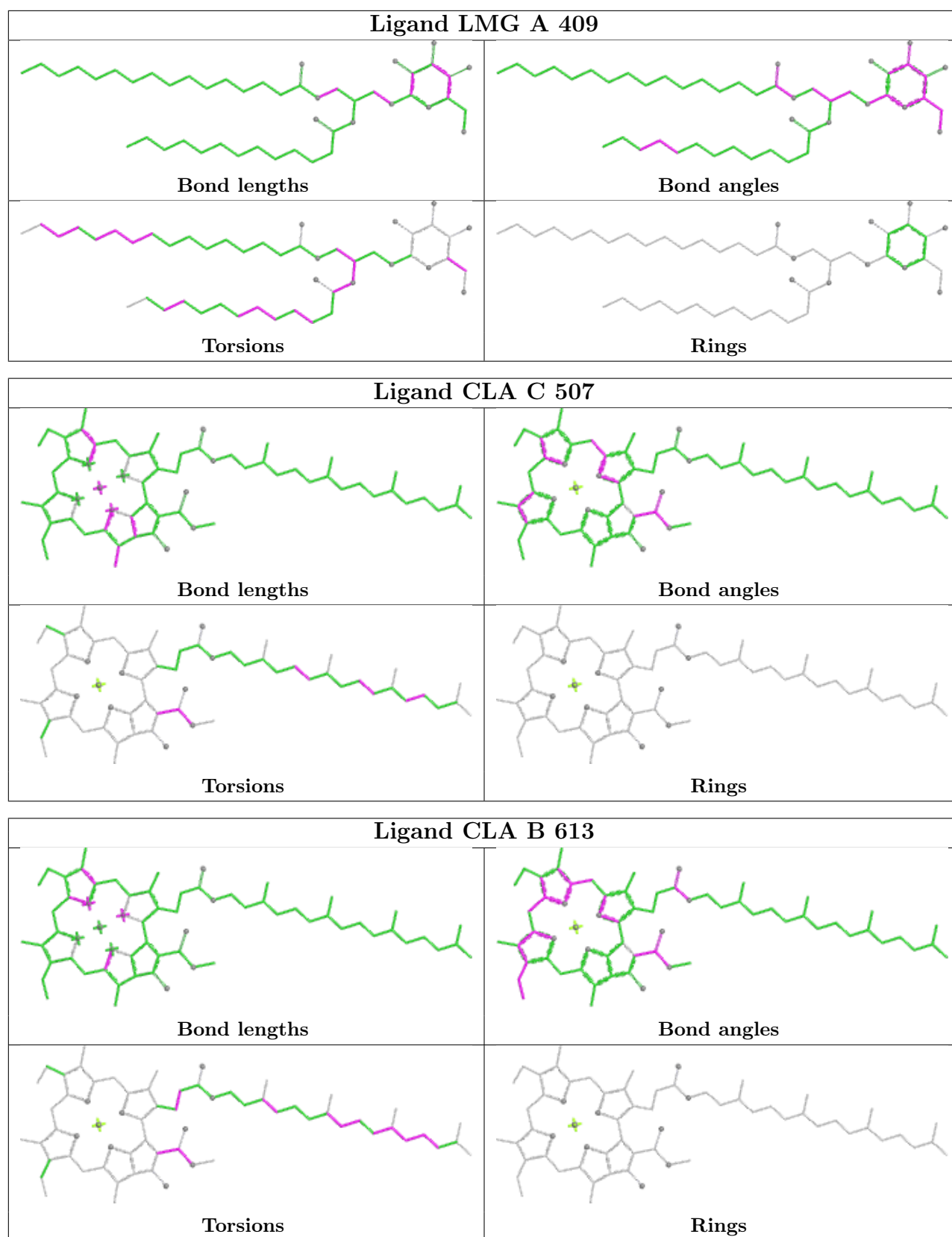


Ligand STE C 519

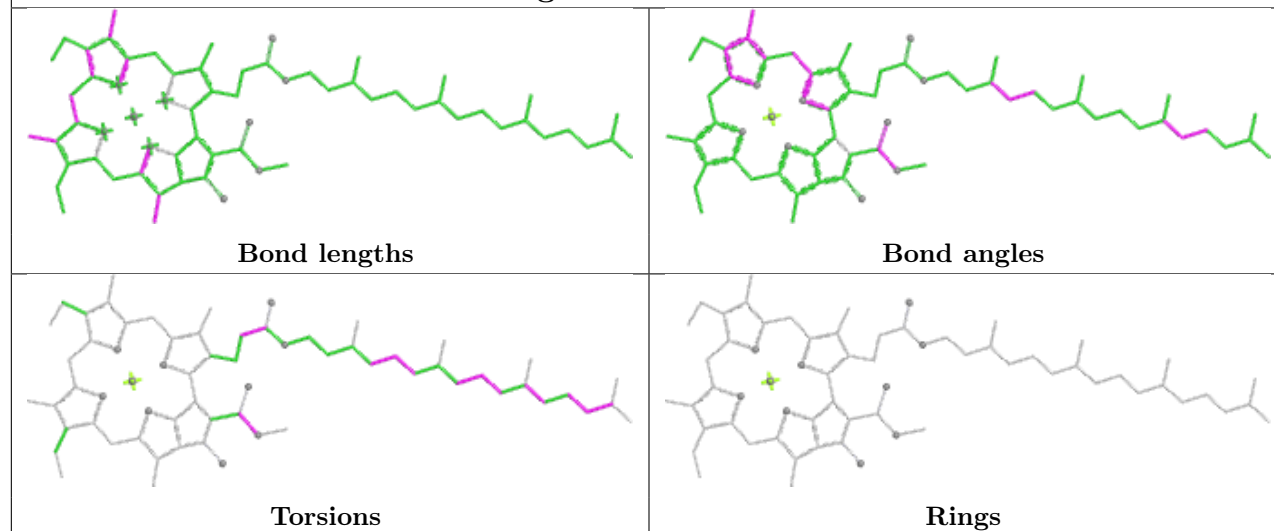


Ligand LMG b 622	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA c 513	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

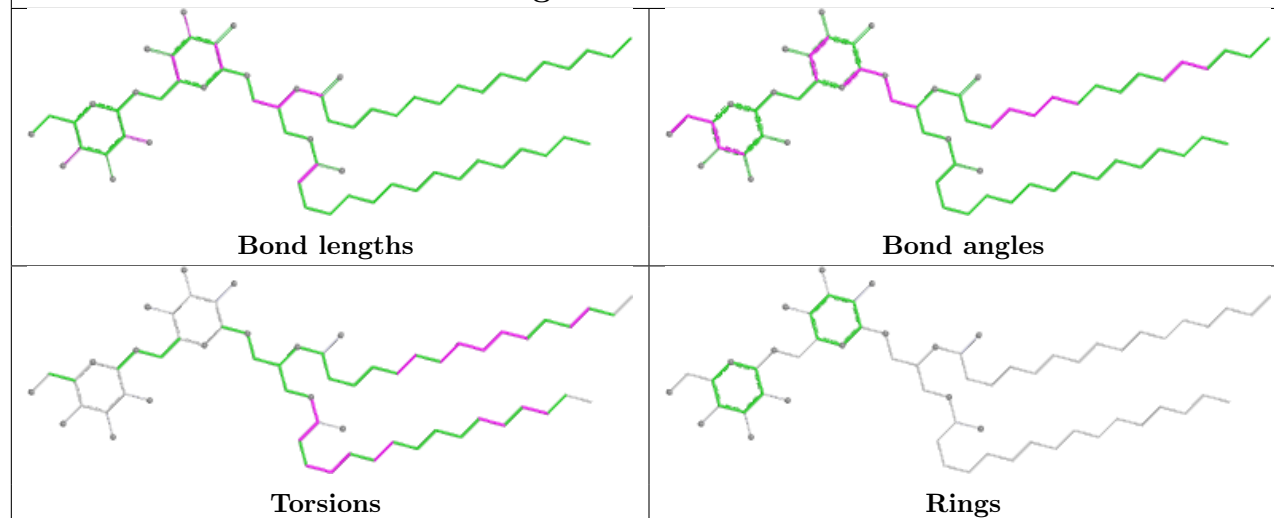




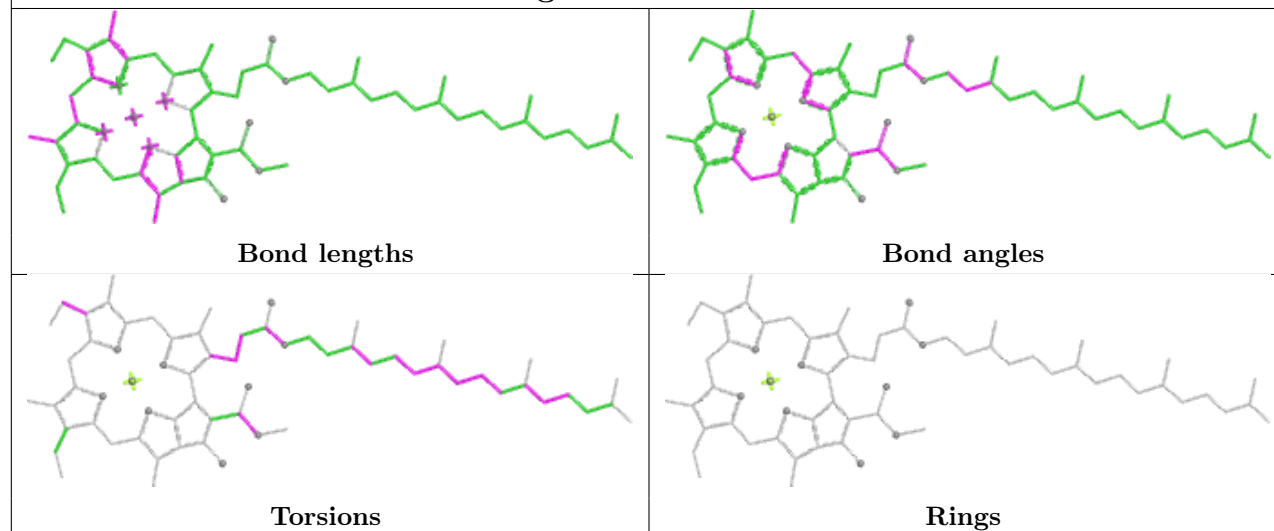
Ligand CLA c 510

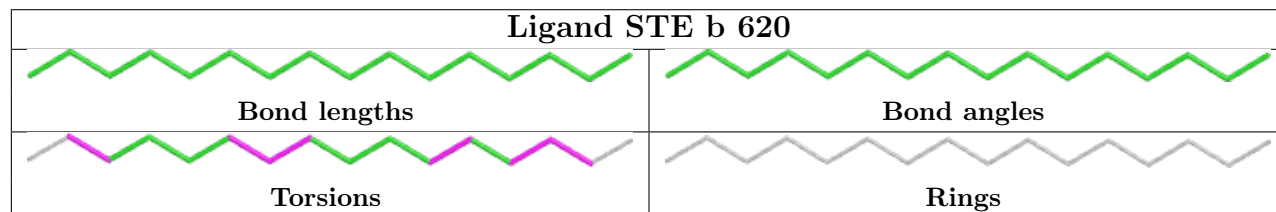
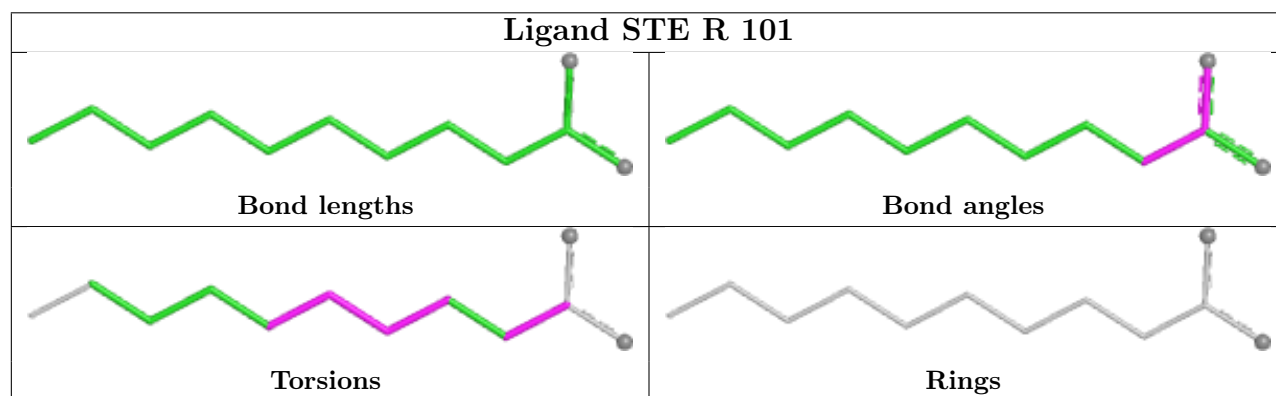
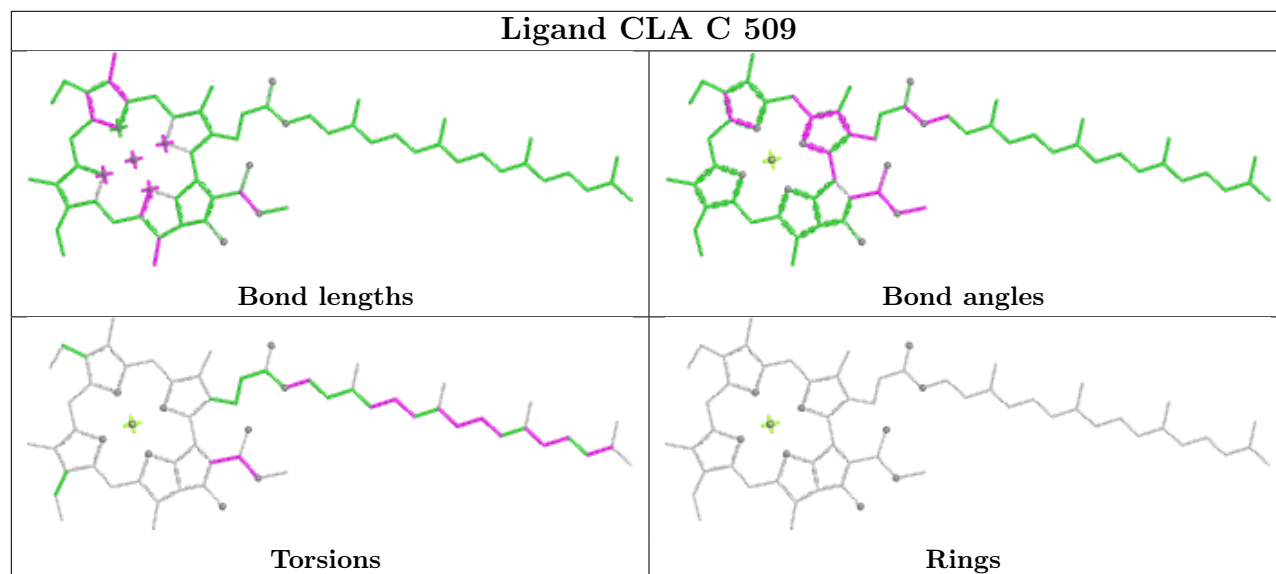
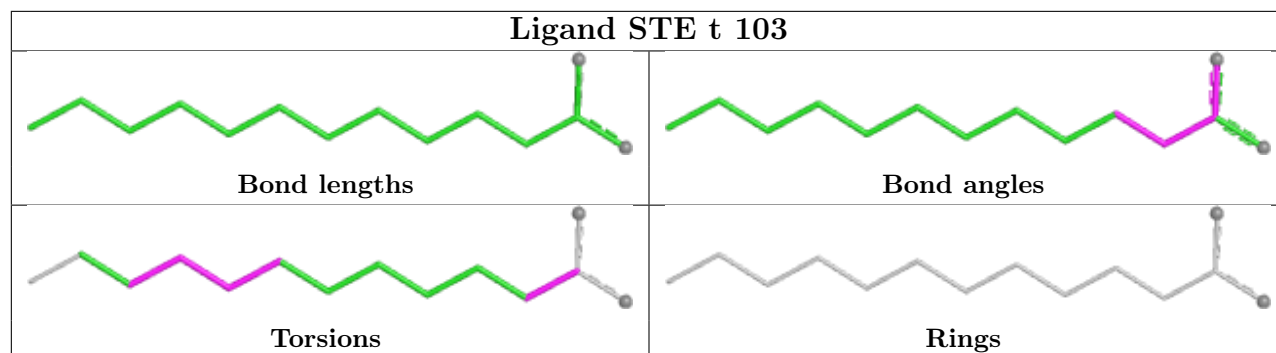


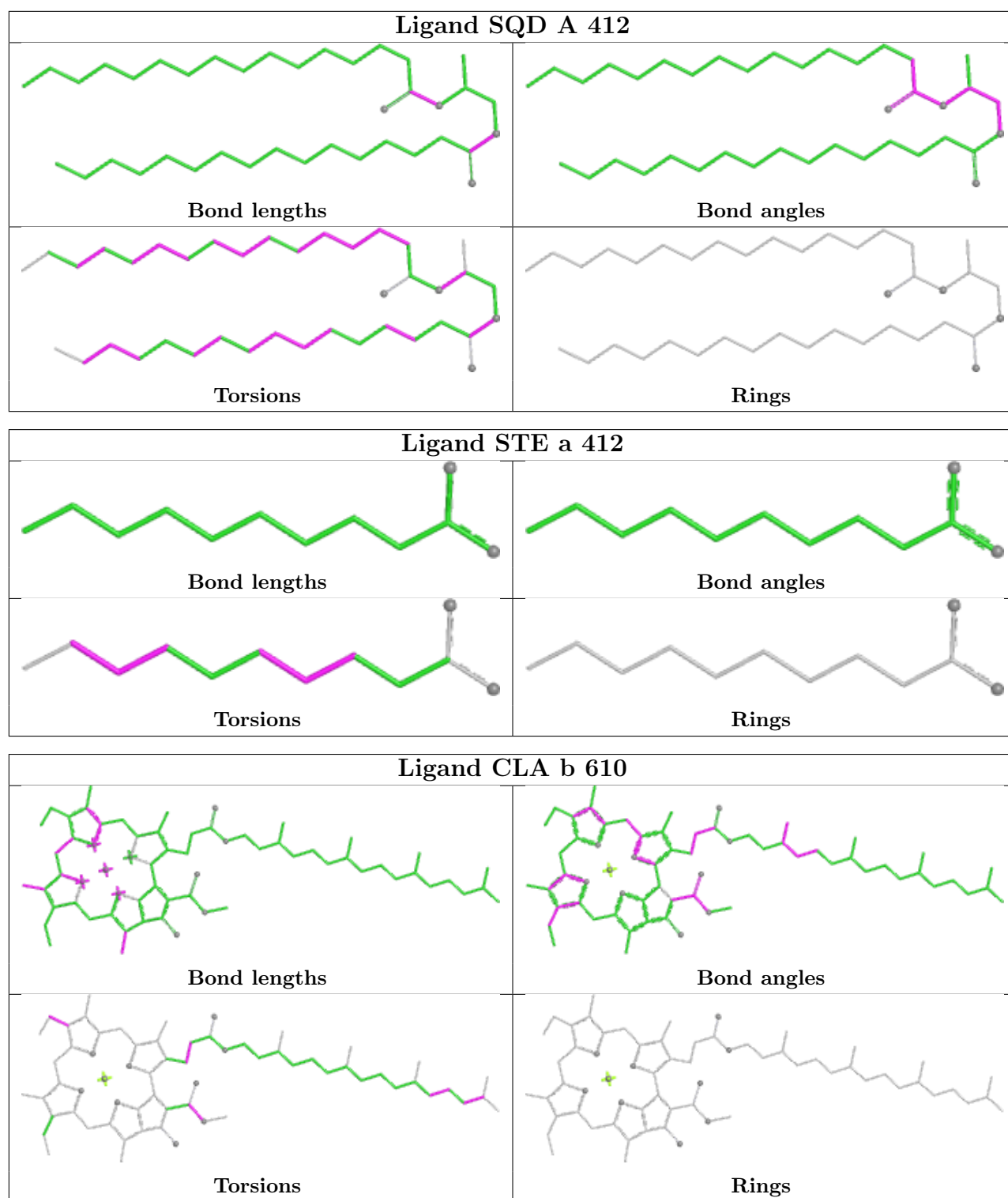
Ligand DGD c 517

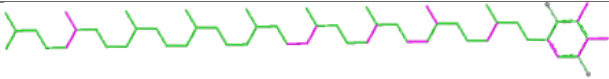
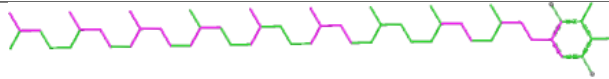
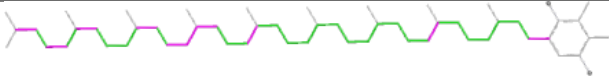
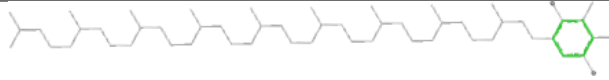


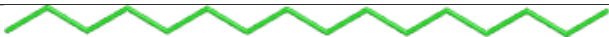
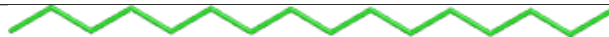
Ligand CLA c 512

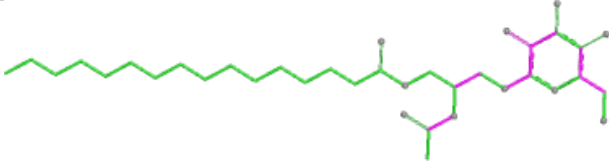
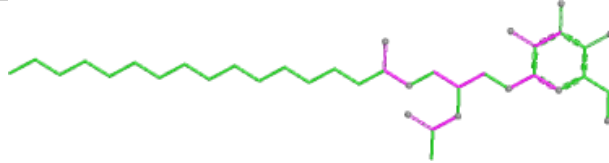
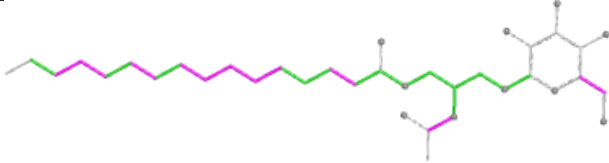
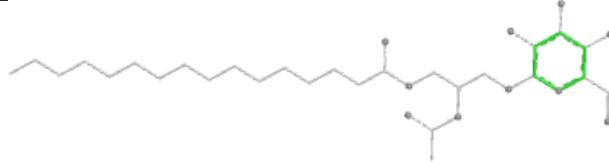






Ligand PL9 D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE B 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG c 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	468:SER	C	469:MET	N	1.17

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.56	0 100 100	28, 38, 58, 91	0
1	a	334/344 (97%)	-0.46	2 (0%) 85 86	29, 40, 69, 87	0
2	B	505/506 (99%)	-0.43	0 100 100	22, 42, 74, 101	4 (0%)
2	b	505/506 (99%)	-0.31	4 (0%) 82 84	31, 46, 83, 115	0
3	C	442/461 (95%)	-0.37	0 100 100	22, 46, 64, 94	1 (0%)
3	c	451/461 (97%)	-0.29	1 (0%) 91 91	25, 50, 75, 112	2 (0%)
4	D	341/352 (96%)	-0.53	0 100 100	29, 40, 59, 95	0
4	d	341/352 (96%)	-0.39	0 100 100	29, 43, 68, 94	1 (0%)
5	E	82/84 (97%)	0.03	2 (2%) 59 61	34, 62, 81, 88	1 (1%)
5	e	82/84 (97%)	0.18	1 (1%) 76 78	47, 73, 91, 100	0
6	F	34/45 (75%)	-0.30	0 100 100	44, 54, 74, 88	0
6	f	34/45 (75%)	-0.15	0 100 100	51, 60, 88, 106	0
7	H	65/66 (98%)	-0.26	1 (1%) 72 73	40, 51, 72, 78	0
7	h	63/66 (95%)	0.04	2 (3%) 50 52	48, 63, 74, 87	0
8	I	35/38 (92%)	-0.32	1 (2%) 53 55	39, 49, 80, 95	0
8	i	35/38 (92%)	-0.18	0 100 100	38, 50, 85, 94	0
9	J	36/40 (90%)	-0.13	0 100 100	44, 60, 85, 100	0
9	j	36/40 (90%)	0.04	0 100 100	49, 64, 100, 119	0
10	K	37/46 (80%)	-0.19	0 100 100	49, 63, 80, 86	0
10	k	37/46 (80%)	0.06	0 100 100	60, 68, 85, 92	0
11	L	37/37 (100%)	-0.64	0 100 100	33, 39, 73, 83	0
11	l	36/37 (97%)	-0.57	0 100 100	32, 41, 86, 93	0
12	M	32/36 (88%)	-0.43	0 100 100	37, 45, 73, 84	0
12	m	31/36 (86%)	-0.48	0 100 100	37, 44, 61, 88	0

Continued on next page...

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.23	2 (0%) 82 84	30, 52, 96, 138	1 (0%)
13	o	244/272 (89%)	-0.27	2 (0%) 82 84	31, 50, 90, 145	0
14	R	34/41 (82%)	0.61	1 (2%) 53 55	70, 83, 103, 108	0
14	r	31/41 (75%)	1.23	5 (16%) 4 5	88, 109, 130, 145	0
15	T	29/30 (96%)	-0.57	0 100 100	32, 40, 75, 96	0
15	t	29/30 (96%)	-0.39	1 (3%) 48 50	35, 41, 92, 97	0
16	U	97/134 (72%)	-0.20	0 100 100	36, 54, 81, 106	0
16	u	97/134 (72%)	-0.31	0 100 100	39, 52, 68, 83	0
17	V	137/163 (84%)	-0.42	0 100 100	34, 50, 65, 87	0
17	v	137/163 (84%)	-0.20	0 100 100	40, 58, 84, 91	0
18	X	38/41 (92%)	-0.11	1 (2%) 57 59	51, 62, 87, 98	0
18	x	39/41 (95%)	0.06	1 (2%) 57 59	58, 69, 98, 118	0
19	Y	27/46 (58%)	0.78	3 (11%) 10 11	64, 87, 104, 113	0
19	y	30/46 (65%)	0.54	1 (3%) 49 51	73, 87, 100, 117	0
20	Z	62/62 (100%)	0.48	2 (3%) 50 52	63, 79, 130, 143	0
20	z	62/62 (100%)	0.54	3 (4%) 35 36	70, 87, 124, 133	0
All	All	5302/5688 (93%)	-0.29	36 (0%) 84 85	22, 48, 87, 145	10 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	4.6
15	t	30	THR	4.5
20	z	33	TRP	3.9
18	x	40	SER	3.4
14	R	35	LEU	3.3
5	E	3	GLY	3.3
5	e	79	PHE	2.9
14	r	20	VAL	2.8
7	h	64	ALA	2.8
14	r	32	GLN	2.7
20	Z	62	VAL	2.6
5	E	79	PHE	2.6
14	r	14	LEU	2.5
20	Z	30	PRO	2.5
20	z	27	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
19	Y	22	LEU	2.5
2	b	133	LEU	2.4
8	I	36	ASP	2.4
2	b	495	PHE	2.4
14	r	3	TRP	2.4
1	a	248	ILE	2.3
1	a	250	ALA	2.3
19	Y	20	ALA	2.3
18	X	2	THR	2.3
13	O	60	ARG	2.3
2	b	84	THR	2.3
7	h	21	VAL	2.3
3	c	23	ALA	2.2
20	z	30	PRO	2.2
19	Y	25	ILE	2.2
13	o	57	LYS	2.2
13	O	221	SER	2.2
19	y	45	ASN	2.1
2	b	494	GLY	2.1
14	r	9	LEU	2.1
7	H	41	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	I	1	10/11	0.93	0.10	46,62,75,90	0
12	FME	M	1	10/11	0.95	0.09	44,61,78,87	0
12	FME	m	1	10/11	0.95	0.09	46,57,89,91	0
15	FME	T	1	10/11	0.95	0.09	30,62,79,79	0
15	FME	t	1	10/11	0.96	0.07	33,54,70,73	0
8	FME	i	1	10/11	0.97	0.07	45,59,72,78	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	STE	b	629	20/20	0.76	0.18	40,71,89,93	0
31	STE	b	628	14/20	0.78	0.19	57,77,110,110	0
31	STE	b	627	10/20	0.79	0.16	45,58,65,68	0
31	STE	B	624	16/20	0.79	0.17	43,71,87,89	0
31	STE	a	412	12/20	0.79	0.15	46,79,97,98	0
31	STE	k	104	12/20	0.79	0.13	56,73,85,89	0
31	STE	I	102	15/20	0.80	0.16	40,58,82,84	0
28	LHG	a	411	42/49	0.80	0.15	66,95,118,141	0
31	STE	H	104	18/20	0.81	0.15	49,76,90,93	0
31	STE	B	623	18/20	0.82	0.14	54,72,94,94	0
31	STE	b	625	15/20	0.82	0.16	52,68,93,94	0
28	LHG	A	411	49/49	0.82	0.14	50,86,108,119	0
26	LMG	c	520	48/55	0.83	0.14	35,83,112,118	0
31	STE	b	626	20/20	0.83	0.15	43,74,97,100	0
31	STE	c	519	20/20	0.83	0.12	43,66,97,102	0
26	LMG	b	622	55/55	0.83	0.15	48,80,110,117	0
31	STE	b	620	16/20	0.84	0.14	42,55,83,100	0
26	LMG	a	414	55/55	0.85	0.13	40,67,93,105	0
27	SQD	A	412	39/54	0.85	0.14	47,69,107,111	0
22	CLA	b	601	65/65	0.85	0.12	51,74,102,106	0
31	STE	B	625	12/20	0.85	0.14	47,69,89,93	0
31	STE	b	624	16/20	0.85	0.14	53,74,88,95	0
31	STE	C	519	12/20	0.85	0.13	41,55,68,73	0
31	STE	t	104	10/20	0.85	0.15	45,59,73,73	0
31	STE	C	520	16/20	0.86	0.14	43,63,75,79	0
25	PL9	A	408	55/55	0.86	0.14	34,70,94,98	0
31	STE	b	621	20/20	0.86	0.12	44,63,85,87	0
26	LMG	c	518	37/55	0.86	0.12	49,72,93,98	0
31	STE	J	101	12/20	0.86	0.13	51,71,80,81	0
31	STE	M	103	10/20	0.86	0.14	35,56,69,69	0
25	PL9	a	409	55/55	0.87	0.14	42,77,102,105	0
31	STE	R	101	12/20	0.87	0.14	59,80,103,104	0
22	CLA	H	101	65/65	0.87	0.11	36,70,99,108	0
31	STE	j	101	12/20	0.87	0.11	50,63,72,76	0
31	STE	a	413	15/20	0.87	0.16	35,65,81,92	0
31	STE	L	103	12/20	0.87	0.15	49,66,79,86	0
29	DGD	A	413	66/66	0.88	0.10	41,65,89,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	STE	B	619	17/20	0.88	0.12	37,58,76,80	0
31	STE	B	622	12/20	0.88	0.11	36,57,72,72	0
26	LMG	D	412	33/55	0.88	0.13	36,63,101,106	0
31	STE	d	411	17/20	0.88	0.12	49,65,73,79	0
27	SQD	t	102	36/54	0.88	0.13	31,69,96,103	0
26	LMG	Y	101	48/55	0.88	0.11	54,76,95,104	0
26	LMG	B	620	28/55	0.88	0.13	35,52,67,71	0
31	STE	x	102	20/20	0.88	0.12	51,68,91,94	0
27	SQD	f	102	41/54	0.89	0.13	61,87,110,127	0
26	LMG	A	409	48/55	0.89	0.10	36,63,86,104	0
31	STE	M	104	18/20	0.89	0.11	38,53,75,86	0
27	SQD	L	101	49/54	0.89	0.11	40,66,106,121	0
26	LMG	c	521	49/55	0.90	0.11	32,66,98,113	0
31	STE	t	103	14/20	0.90	0.10	41,59,67,71	0
26	LMG	M	101	51/55	0.90	0.10	37,56,84,88	0
27	SQD	B	621	54/54	0.90	0.10	40,67,93,104	0
26	LMG	m	101	51/55	0.91	0.10	40,61,86,96	0
31	STE	C	521	12/20	0.91	0.11	37,48,59,64	0
26	LMG	d	410	44/55	0.91	0.10	41,61,90,108	0
31	STE	Z	101	8/20	0.91	0.12	38,65,78,78	0
30	BCR	k	101	40/40	0.91	0.11	48,67,82,91	0
30	BCR	x	101	40/40	0.91	0.09	40,59,76,81	0
27	SQD	a	410	54/54	0.91	0.11	44,70,104,112	0
22	CLA	c	512	65/65	0.92	0.10	44,62,97,112	0
22	CLA	c	513	65/65	0.92	0.10	44,80,112,121	0
22	CLA	C	513	65/65	0.92	0.10	43,65,107,118	0
30	BCR	C	514	40/40	0.92	0.10	30,47,58,76	0
30	BCR	K	101	40/40	0.92	0.10	45,63,82,83	0
30	BCR	K	102	40/40	0.92	0.09	37,57,74,74	0
30	BCR	d	406	40/40	0.92	0.09	30,58,103,111	0
27	SQD	D	409	36/54	0.92	0.11	50,78,97,114	0
31	STE	X	101	20/20	0.92	0.10	40,60,81,91	0
30	BCR	H	102	40/40	0.93	0.08	35,51,67,75	0
27	SQD	A	410	52/54	0.93	0.10	39,68,101,103	0
29	DGD	C	517	62/66	0.93	0.09	30,57,112,139	0
30	BCR	b	619	40/40	0.93	0.08	24,55,73,87	0
29	DGD	H	103	62/66	0.93	0.09	34,51,67,75	0
29	DGD	c	516	62/66	0.93	0.08	36,61,97,110	0
30	BCR	k	102	40/40	0.93	0.09	46,67,84,86	0
31	STE	M	102	15/20	0.93	0.09	37,54,63,69	0
30	BCR	k	103	40/40	0.93	0.11	45,63,78,85	0
29	DGD	c	517	62/66	0.93	0.10	36,64,94,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	DGD	h	101	62/66	0.93	0.09	35,53,70,78	0
30	BCR	B	617	40/40	0.93	0.08	29,44,57,64	0
30	BCR	B	618	40/40	0.93	0.09	24,48,68,80	0
26	LMG	D	408	51/55	0.93	0.11	34,66,92,114	0
30	BCR	D	406	40/40	0.93	0.09	35,50,88,108	0
22	CLA	c	511	65/65	0.94	0.10	41,62,80,90	0
30	BCR	c	514	40/40	0.94	0.09	35,51,69,74	0
22	CLA	C	512	65/65	0.94	0.09	40,61,96,105	0
22	CLA	C	510	65/65	0.94	0.08	30,50,68,81	0
30	BCR	C	515	40/40	0.94	0.10	42,60,73,75	0
22	CLA	c	506	65/65	0.94	0.09	34,56,106,111	0
28	LHG	b	623	49/49	0.94	0.10	38,58,85,104	0
30	BCR	I	101	40/40	0.94	0.07	22,40,52,54	0
28	LHG	d	409	39/49	0.94	0.09	37,55,73,83	0
30	BCR	B	616	40/40	0.94	0.08	30,46,69,72	0
30	BCR	T	101	40/40	0.94	0.07	30,46,61,66	0
30	BCR	a	406	40/40	0.94	0.07	24,38,59,64	0
30	BCR	b	617	40/40	0.94	0.08	34,48,64,67	0
30	BCR	b	618	40/40	0.94	0.07	29,44,61,68	0
22	CLA	a	405	65/65	0.95	0.08	20,44,90,104	0
22	CLA	C	503	65/65	0.95	0.07	31,49,59,63	0
22	CLA	b	606	65/65	0.95	0.08	29,47,83,90	0
22	CLA	b	609	65/65	0.95	0.08	31,54,74,77	0
22	CLA	b	612	65/65	0.95	0.07	27,40,54,58	0
22	CLA	b	615	65/65	0.95	0.08	27,47,67,74	0
22	CLA	b	616	60/65	0.95	0.09	31,48,93,99	0
22	CLA	c	502	65/65	0.95	0.07	30,49,69,76	0
22	CLA	c	503	65/65	0.95	0.08	34,50,62,68	0
22	CLA	C	506	65/65	0.95	0.08	28,50,90,108	0
22	CLA	c	508	64/65	0.95	0.08	36,56,98,124	0
22	CLA	c	509	65/65	0.95	0.09	32,54,74,84	0
22	CLA	C	508	65/65	0.95	0.08	29,48,112,124	0
22	CLA	C	509	65/65	0.95	0.08	31,51,68,77	0
22	CLA	B	605	65/65	0.95	0.08	29,45,82,98	0
22	CLA	d	405	65/65	0.95	0.08	32,56,101,116	0
23	PHO	D	401	64/64	0.95	0.06	26,39,51,54	0
23	PHO	d	401	64/64	0.95	0.07	25,43,55,67	0
22	CLA	C	511	65/65	0.95	0.09	34,59,80,85	0
28	LHG	D	410	49/49	0.95	0.08	31,47,58,65	0
28	LHG	D	411	47/49	0.95	0.10	27,54,84,95	0
25	PL9	D	407	55/55	0.95	0.07	26,39,57,63	0
22	CLA	B	614	65/65	0.95	0.08	26,42,69,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	BCR	t	101	40/40	0.95	0.06	28,44,55,63	0
25	PL9	d	407	55/55	0.95	0.07	25,40,54,60	0
22	CLA	B	615	60/65	0.95	0.09	23,43,96,105	0
29	DGD	C	516	62/66	0.95	0.10	28,48,85,107	0
22	CLA	C	502	65/65	0.95	0.07	29,48,70,79	0
29	DGD	C	518	62/66	0.95	0.08	33,57,77,94	0
22	CLA	a	403	65/65	0.95	0.09	29,47,106,117	0
33	BCT	d	402	4/4	0.95	0.08	35,40,52,62	0
22	CLA	d	404	65/65	0.96	0.07	22,37,47,53	0
28	LHG	D	413	49/49	0.96	0.08	32,48,80,93	0
22	CLA	C	504	59/65	0.96	0.08	30,49,95,100	0
23	PHO	A	404	64/64	0.96	0.06	15,35,45,47	0
28	LHG	d	408	49/49	0.96	0.08	28,48,60,65	0
22	CLA	C	505	65/65	0.96	0.08	27,47,75,82	0
28	LHG	l	101	49/49	0.96	0.08	34,50,65,71	0
23	PHO	a	404	64/64	0.96	0.06	24,37,46,47	0
22	CLA	b	602	65/65	0.96	0.08	31,48,68,71	0
22	CLA	b	603	65/65	0.96	0.07	26,43,82,91	0
22	CLA	b	604	65/65	0.96	0.08	24,45,87,105	0
22	CLA	b	605	65/65	0.96	0.07	24,39,59,63	0
29	DGD	c	515	62/66	0.96	0.08	31,49,85,92	0
22	CLA	B	609	65/65	0.96	0.07	25,39,49,58	0
22	CLA	b	608	65/65	0.96	0.07	30,48,73,79	0
22	CLA	C	507	65/65	0.96	0.07	25,46,67,73	0
22	CLA	b	610	65/65	0.96	0.07	28,43,58,69	0
22	CLA	b	611	65/65	0.96	0.07	25,41,55,66	0
22	CLA	B	610	65/65	0.96	0.06	19,38,54,62	0
22	CLA	b	613	65/65	0.96	0.08	21,41,83,97	0
22	CLA	b	614	65/65	0.96	0.07	26,43,87,93	0
22	CLA	B	611	65/65	0.96	0.07	22,37,50,60	0
22	CLA	B	612	65/65	0.96	0.07	21,40,75,84	0
22	CLA	c	501	65/65	0.96	0.07	30,50,65,68	0
22	CLA	B	613	65/65	0.96	0.08	26,45,87,104	0
22	CLA	B	603	65/65	0.96	0.07	25,40,97,105	0
22	CLA	c	504	60/65	0.96	0.07	36,51,85,99	0
22	CLA	c	505	65/65	0.96	0.08	30,47,73,77	0
22	CLA	B	604	65/65	0.96	0.07	21,38,53,63	0
22	CLA	c	507	65/65	0.96	0.07	31,50,65,78	0
22	CLA	D	403	65/65	0.96	0.06	22,36,53,65	0
22	CLA	D	404	65/65	0.96	0.07	22,35,57,66	0
22	CLA	c	510	65/65	0.96	0.07	36,51,66,92	0
22	CLA	A	402	65/65	0.96	0.06	19,33,52,62	0

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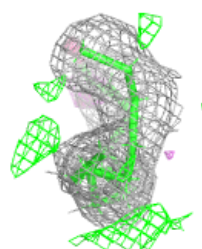
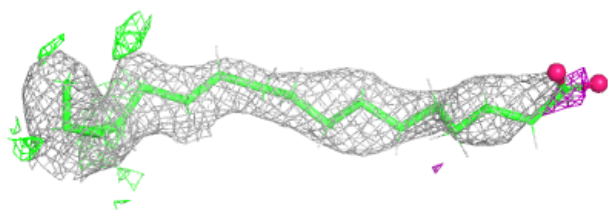
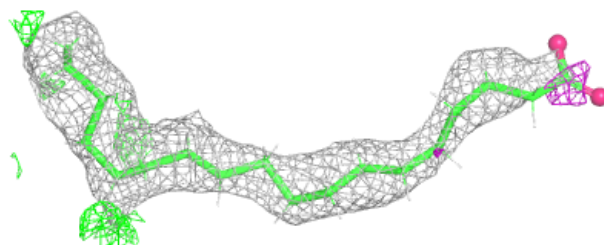
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	a	402	65/65	0.96	0.07	24,36,51,59	0
22	CLA	B	608	65/65	0.96	0.07	27,43,60,65	0
22	CLA	d	403	65/65	0.96	0.08	25,41,70,83	0
34	HEC	f	101	43/43	0.96	0.09	44,62,87,99	0
22	CLA	B	601	65/65	0.97	0.07	26,42,63,67	0
22	CLA	b	607	65/65	0.97	0.07	26,42,86,96	0
22	CLA	B	606	65/65	0.97	0.07	18,39,81,92	0
22	CLA	B	607	65/65	0.97	0.06	27,43,71,75	0
22	CLA	B	602	65/65	0.97	0.07	23,38,67,75	0
22	CLA	A	403	65/65	0.97	0.09	23,42,94,109	0
28	LHG	L	102	49/49	0.97	0.07	30,47,67,80	0
22	CLA	C	501	65/65	0.97	0.06	25,43,59,65	0
33	BCT	D	402	4/4	0.97	0.08	28,35,46,55	0
22	CLA	D	405	65/65	0.97	0.08	26,50,132,139	0
34	HEC	F	101	43/43	0.97	0.07	37,54,73,76	0
22	CLA	A	405	54/65	0.97	0.06	22,36,72,78	0
35	NA	V	202	1/1	0.97	0.10	61,61,61,61	0
24	CL	A	407	1/1	0.98	0.04	39,39,39,39	0
34	HEC	v	201	43/43	0.98	0.07	31,42,53,61	0
34	HEC	V	201	43/43	0.98	0.06	25,39,48,49	0
24	CL	a	407	1/1	0.99	0.03	34,34,34,34	0
24	CL	a	408	1/1	0.99	0.07	35,35,35,35	0
24	CL	A	406	1/1	0.99	0.04	35,35,35,35	0
32	OEX	C	522	10/10	0.99	0.03	26,33,37,38	0
32	OEX	a	415	10/10	0.99	0.03	26,34,36,40	0
21	FE2	A	401	1/1	0.99	0.03	32,32,32,32	0
21	FE2	a	401	1/1	1.00	0.02	36,36,36,36	0

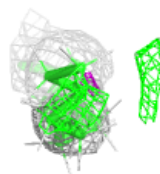
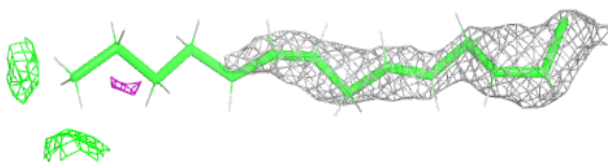
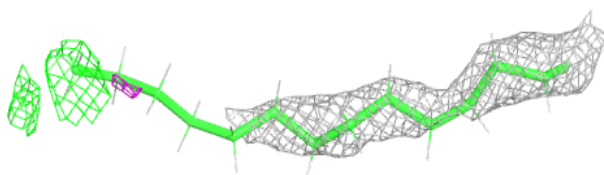
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around STE b 629:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

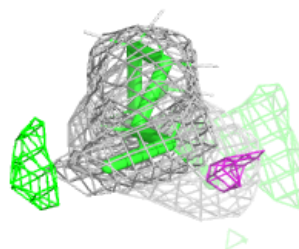
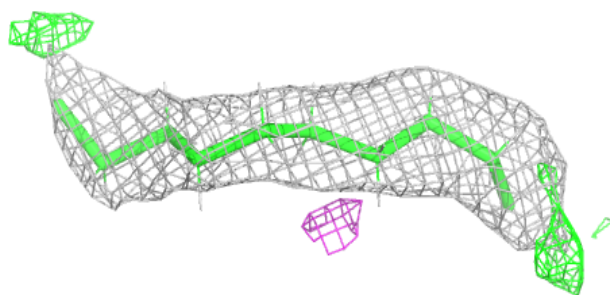
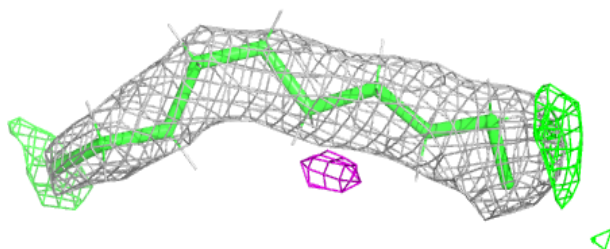
**Electron density around STE b 628:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

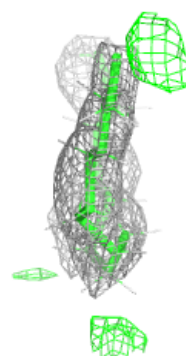
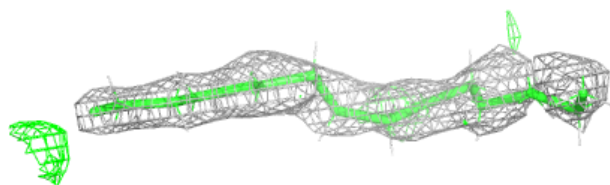
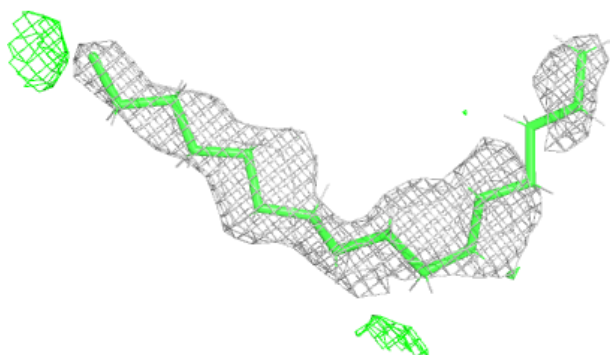


Electron density around STE b 627:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

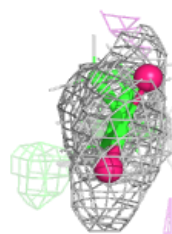
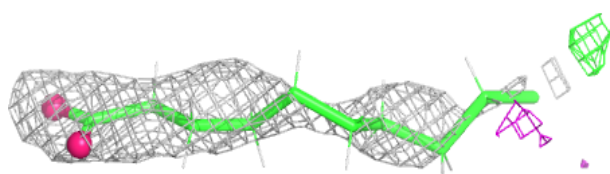
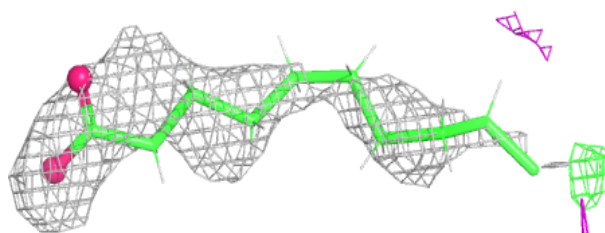
**Electron density around STE B 624:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

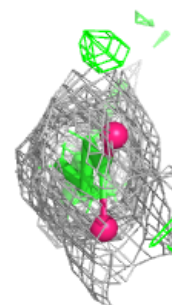
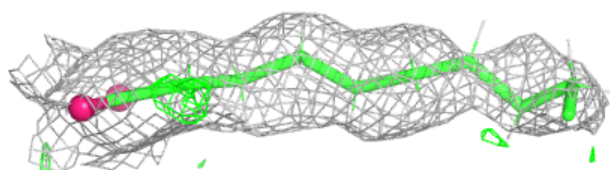
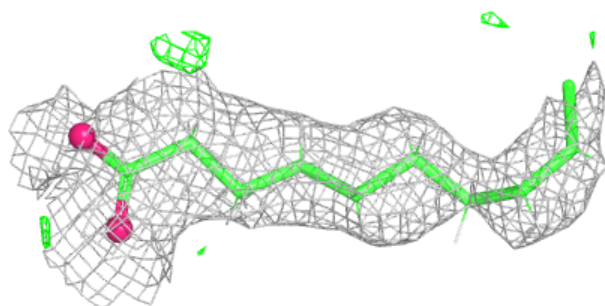


Electron density around STE a 412:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

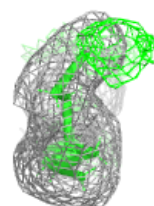
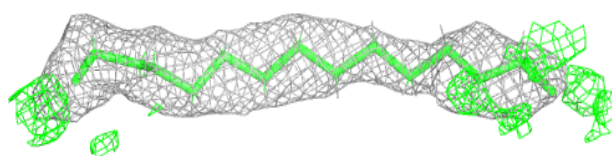
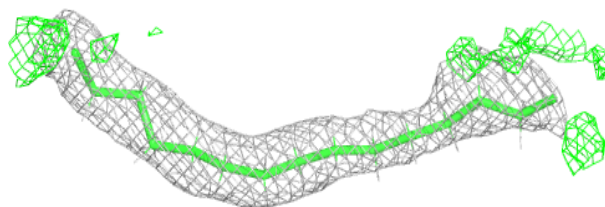
**Electron density around STE k 104:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

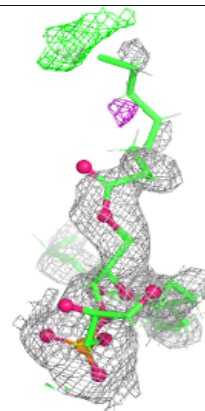
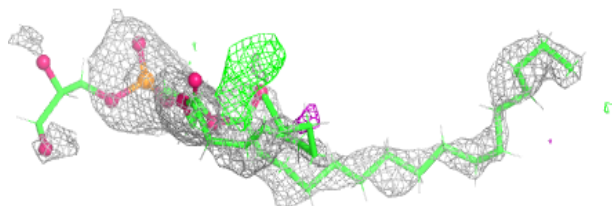
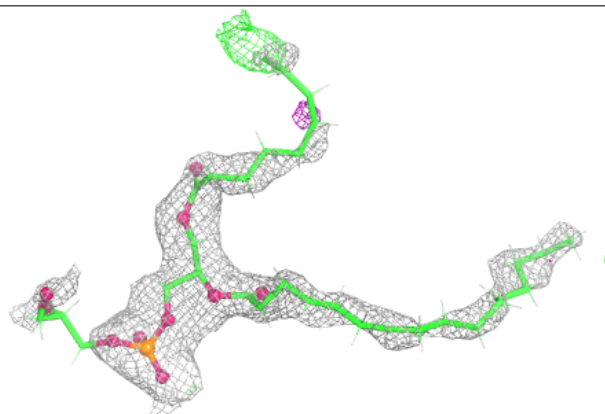


Electron density around STE I 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

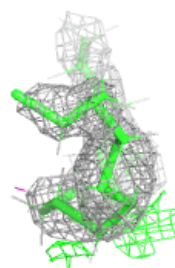
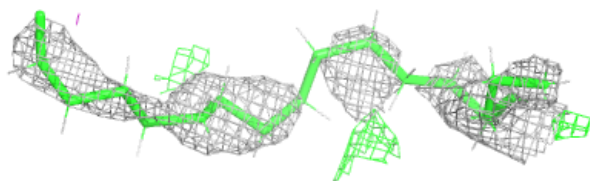
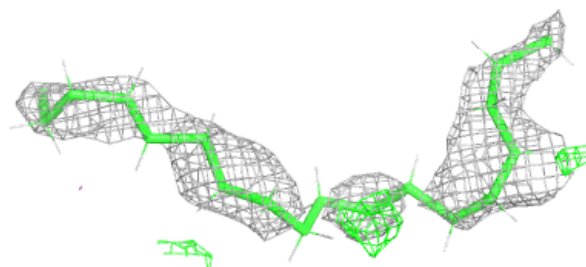
**Electron density around LHG a 411:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

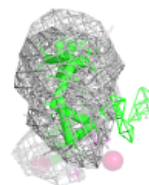
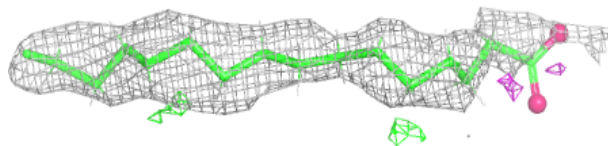
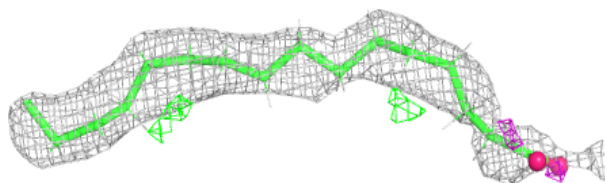


Electron density around STE H 104:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

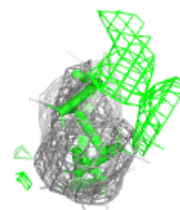
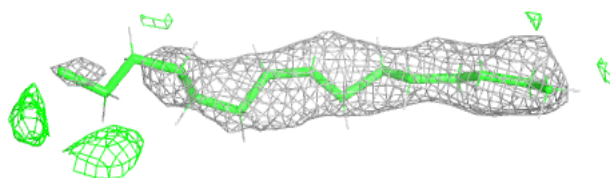
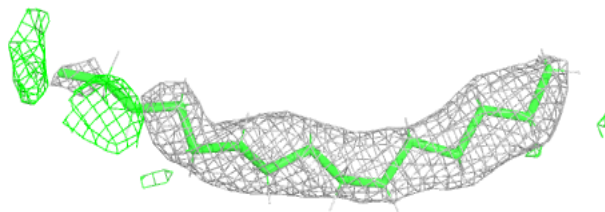
**Electron density around STE B 623:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



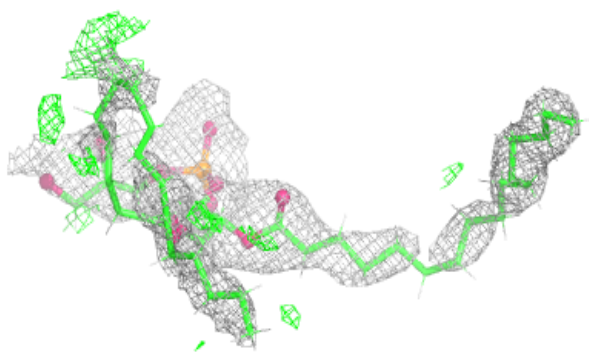
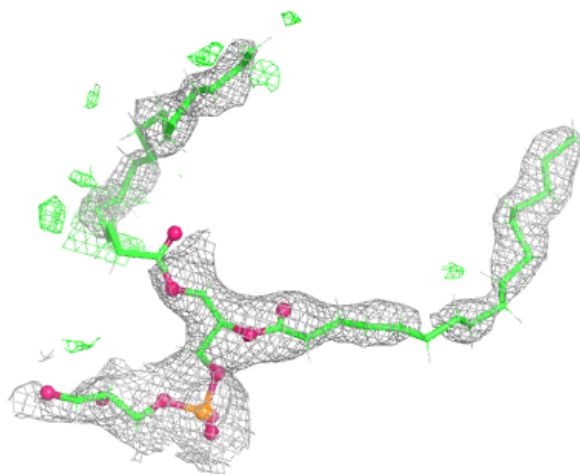
Electron density around STE b 625:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



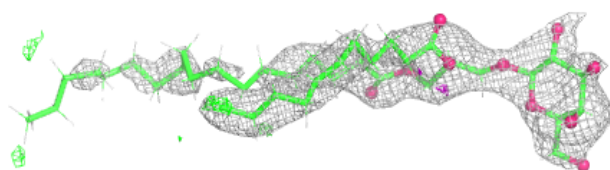
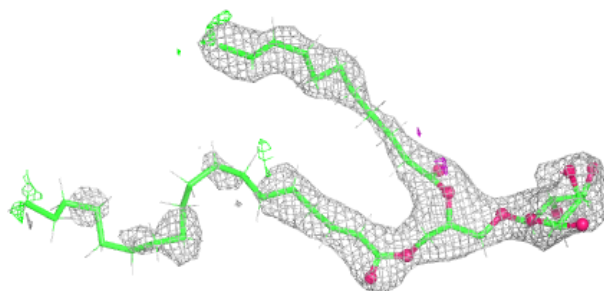
Electron density around LHG A 411:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

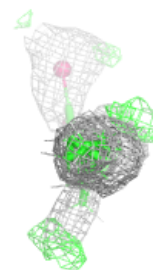
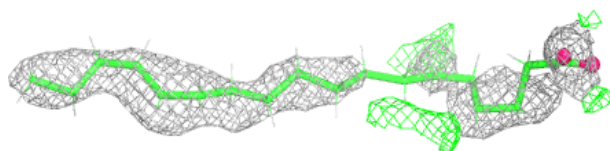
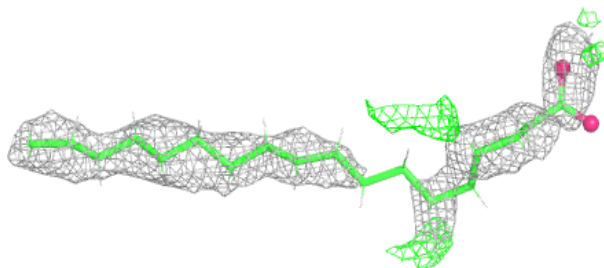


Electron density around LMG c 520:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

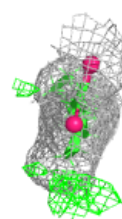
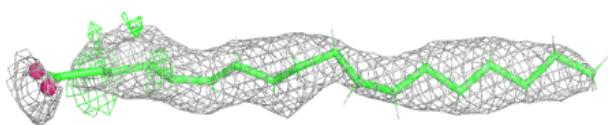
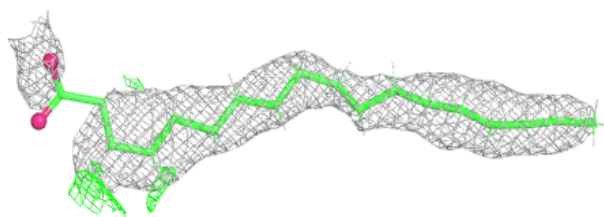
**Electron density around STE b 626:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

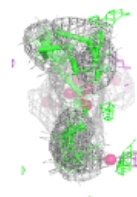
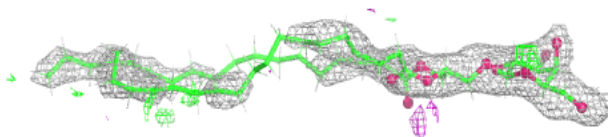
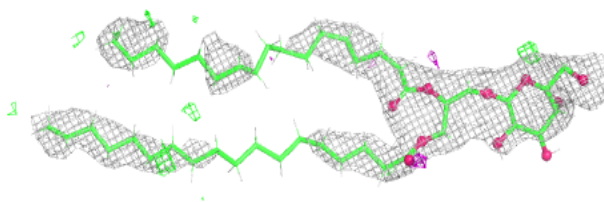


Electron density around STE c 519:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

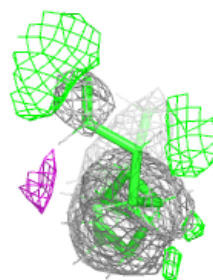
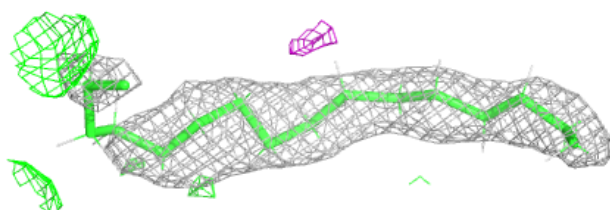
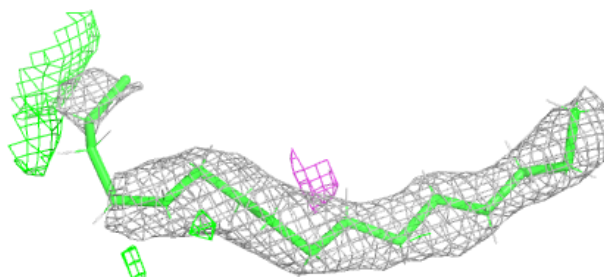
**Electron density around LMG b 622:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

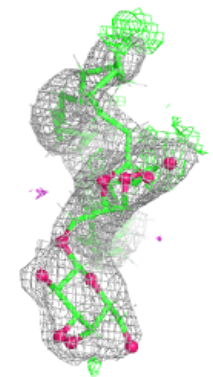
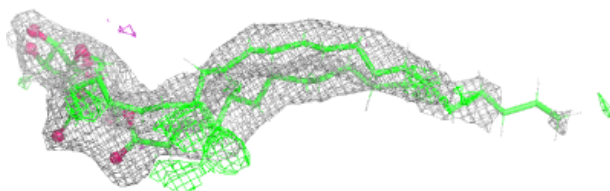
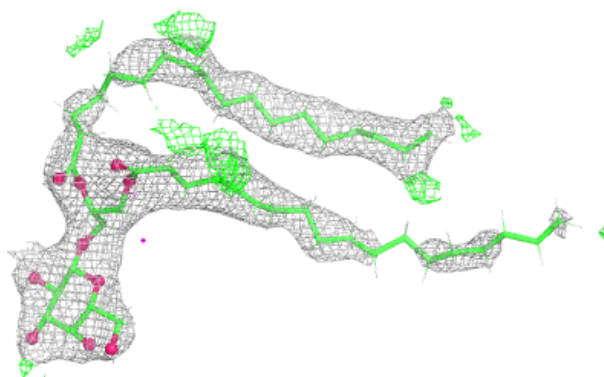


Electron density around STE b 620:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

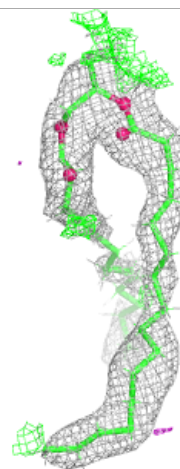
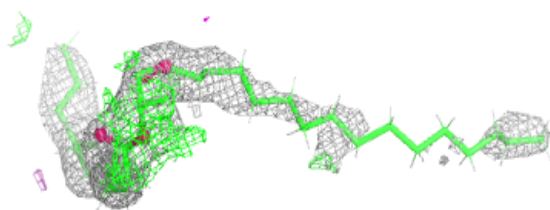
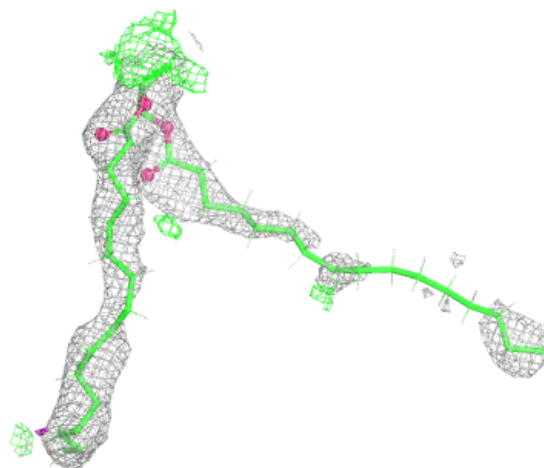
**Electron density around LMG a 414:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



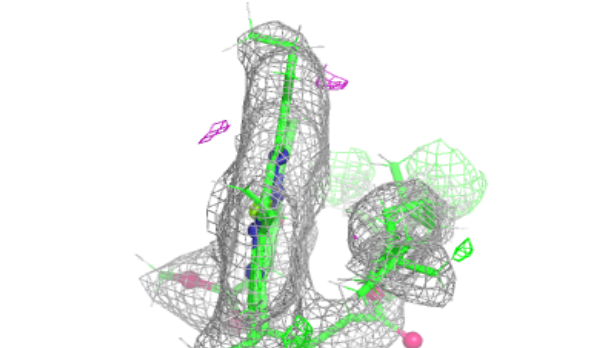
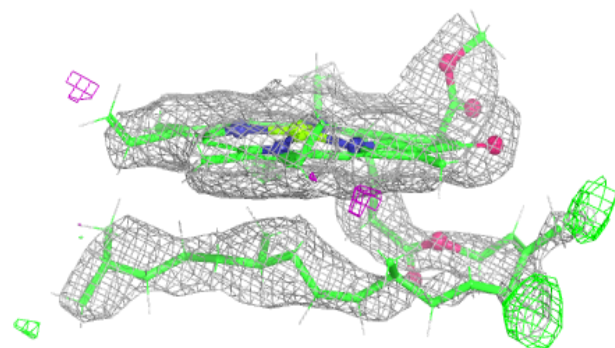
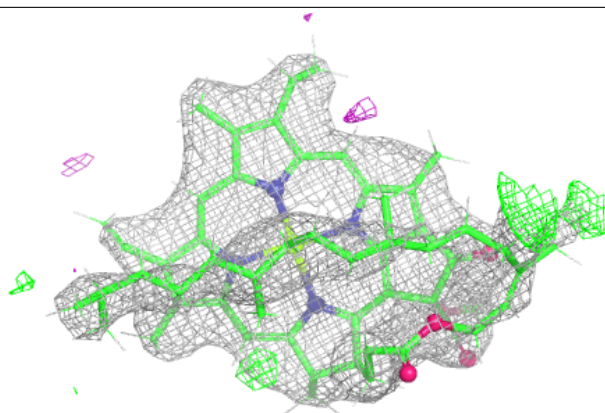
Electron density around SQD A 412:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

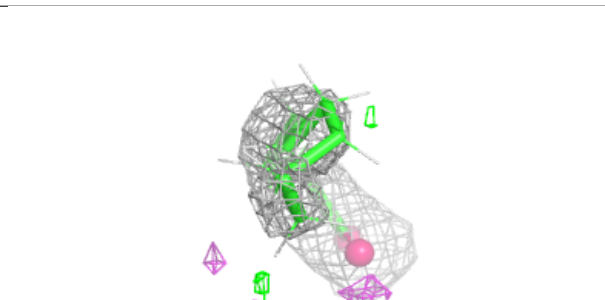
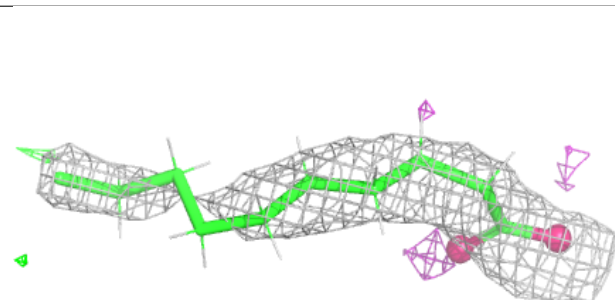
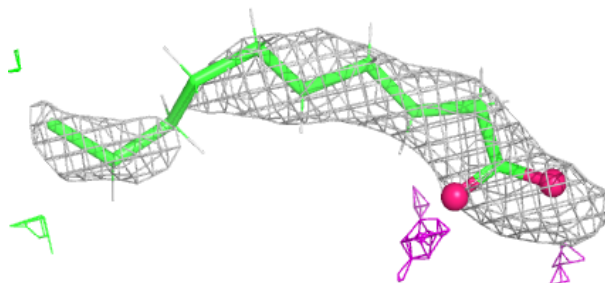


Electron density around CLA b 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

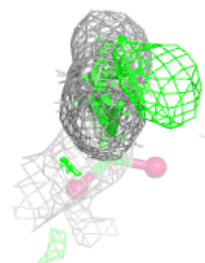
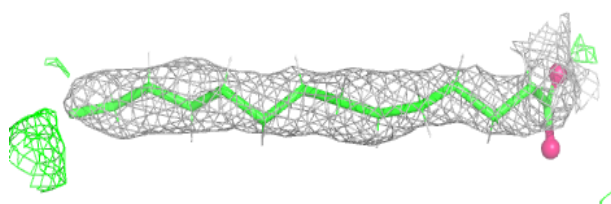
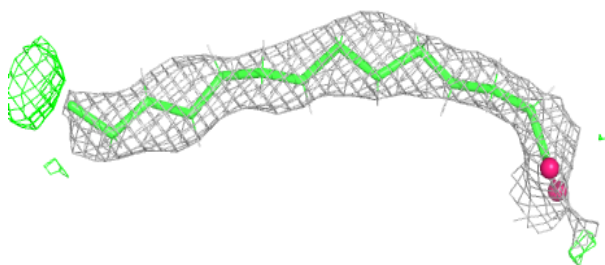
**Electron density around STE B 625:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

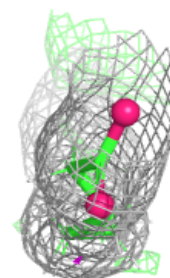
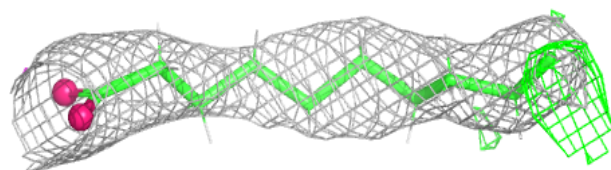
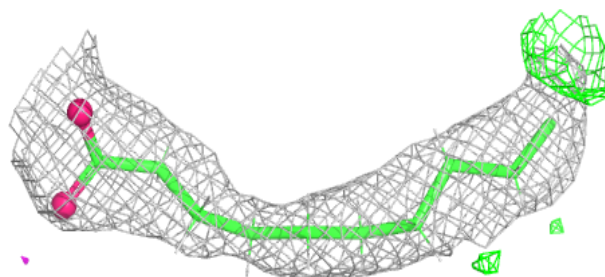


Electron density around STE b 624:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

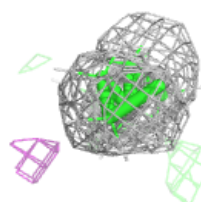
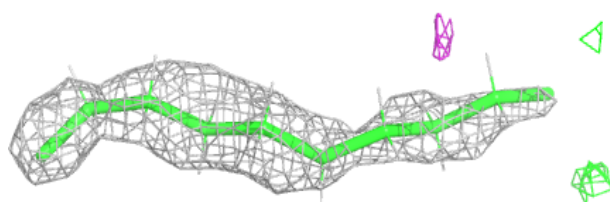
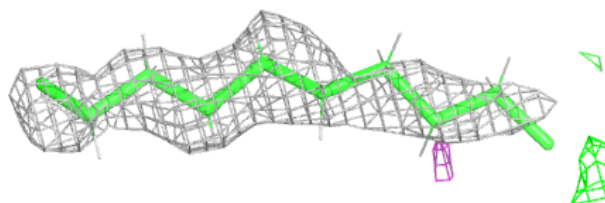
**Electron density around STE C 519:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

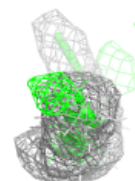
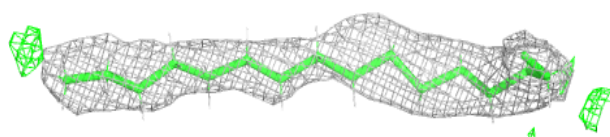
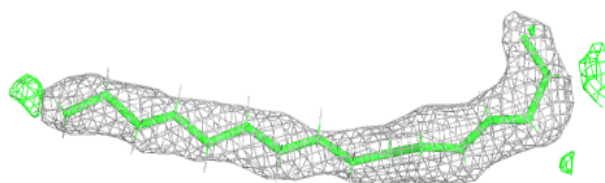


Electron density around STE t 104:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

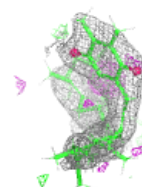
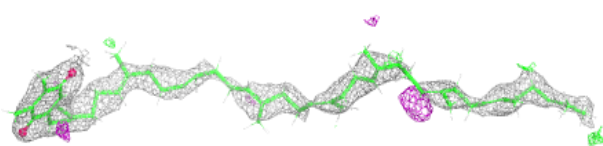
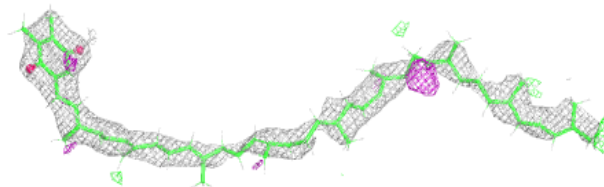
**Electron density around STE C 520:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

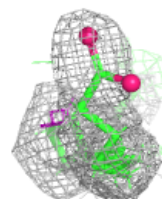
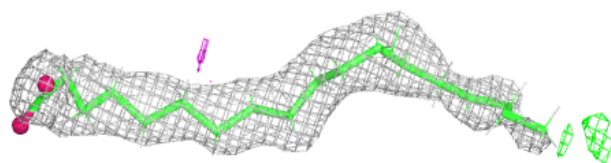
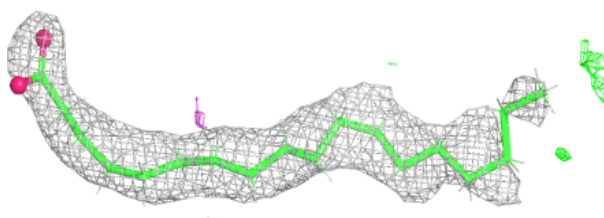


Electron density around PL9 A 408:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

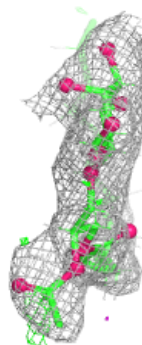
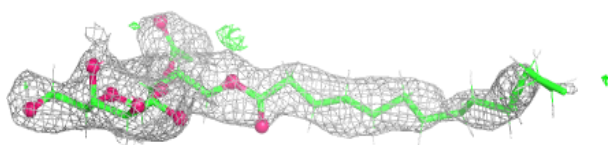
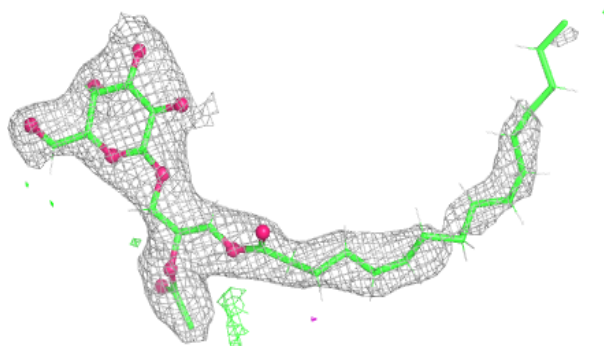
**Electron density around STE b 621:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

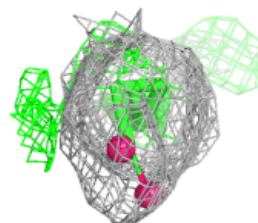
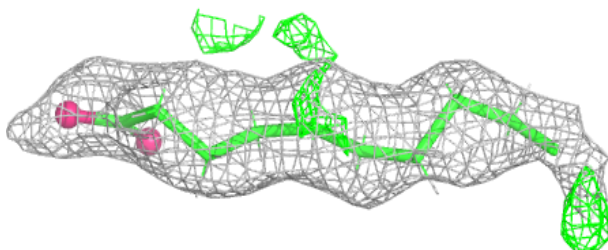
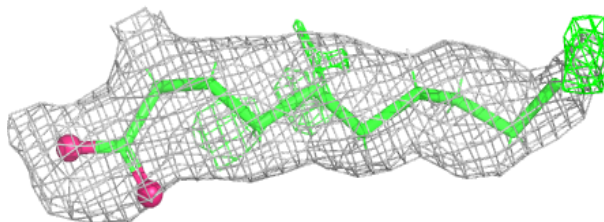


Electron density around LMG c 518:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

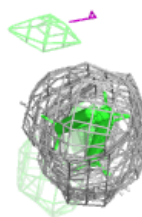
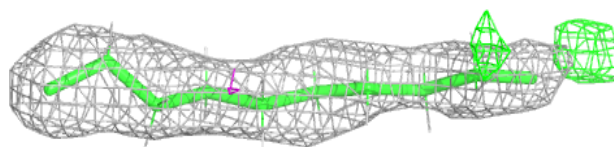
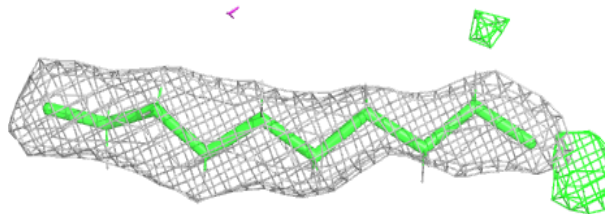
**Electron density around STE J 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

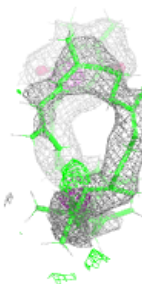
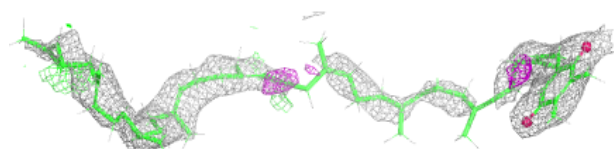
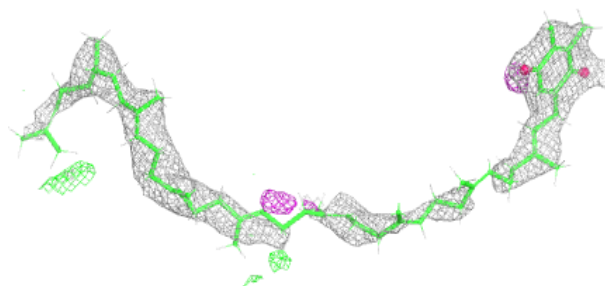


Electron density around STE M 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

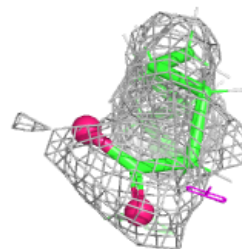
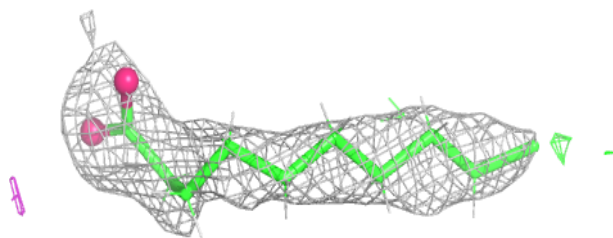
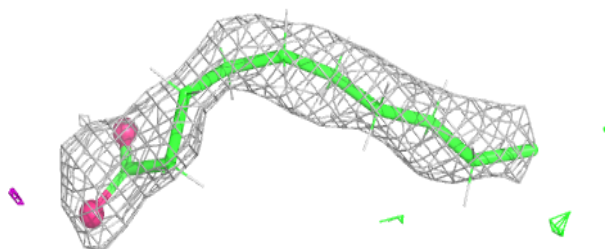
**Electron density around PL9 a 409:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

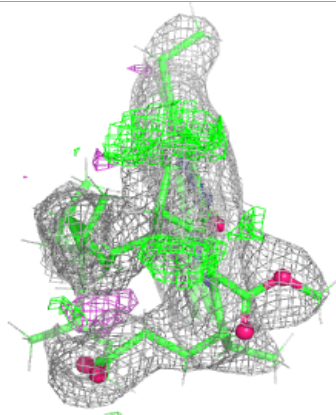
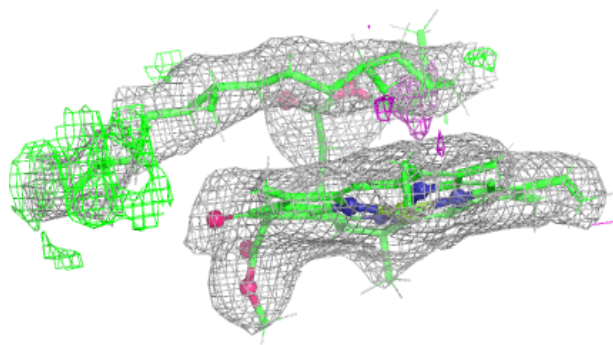
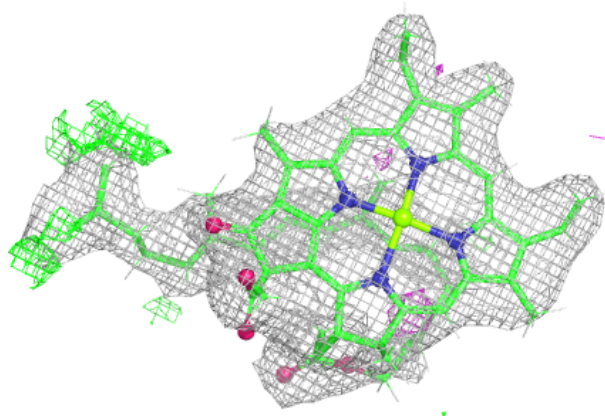


Electron density around STE R 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

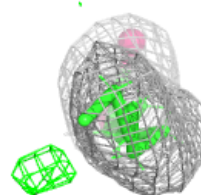
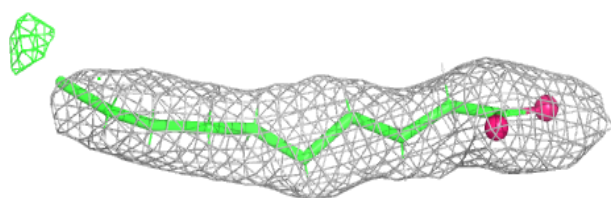
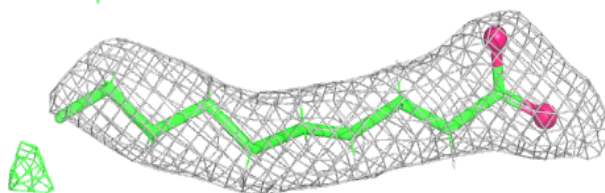
**Electron density around CLA H 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

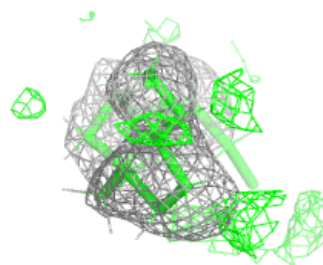
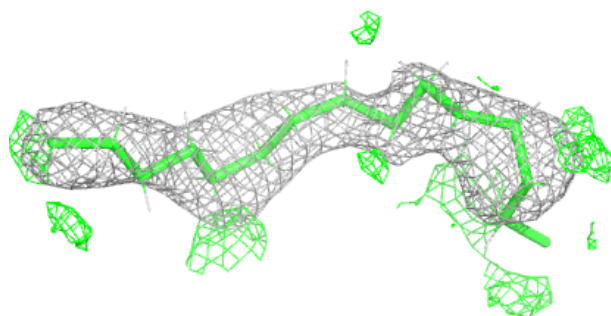
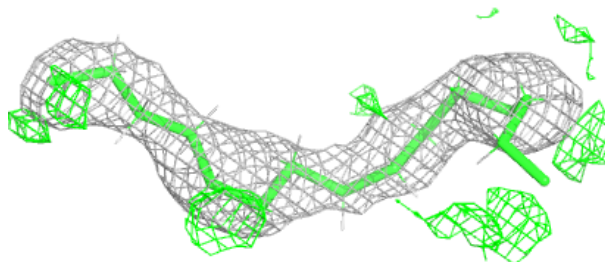


Electron density around STE j 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

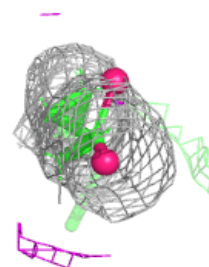
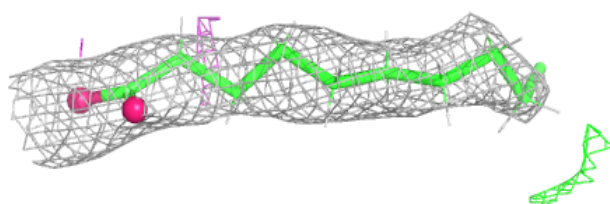
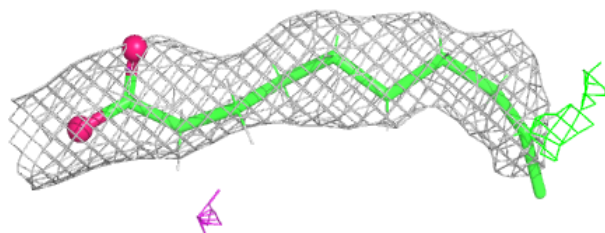
**Electron density around STE a 413:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

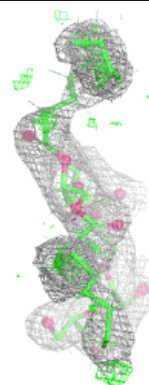
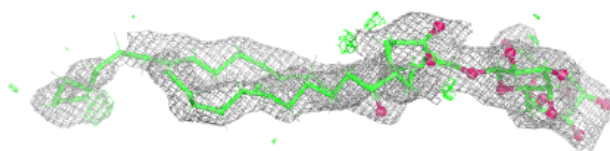
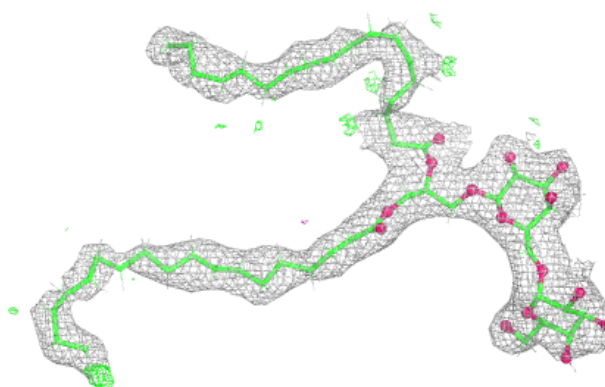


Electron density around STE L 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

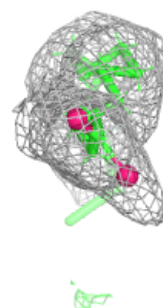
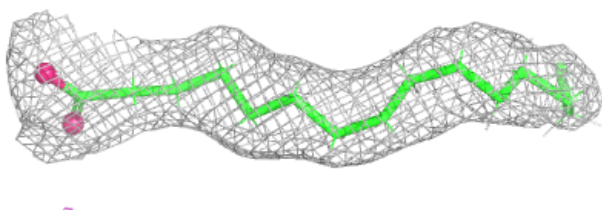
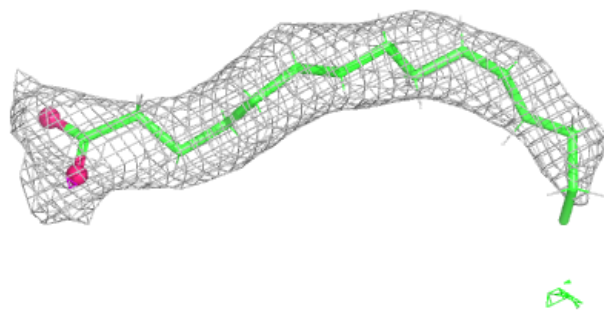
**Electron density around DGD A 413:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

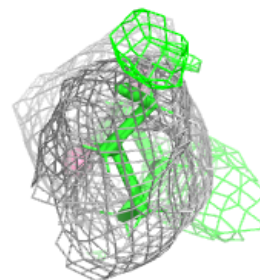
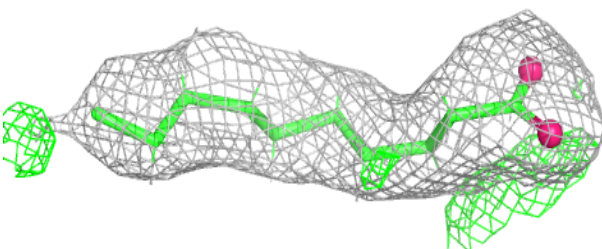
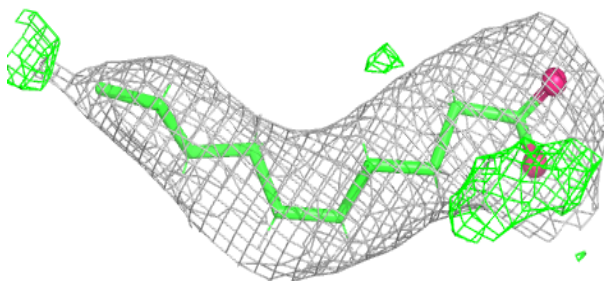


Electron density around STE B 619:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

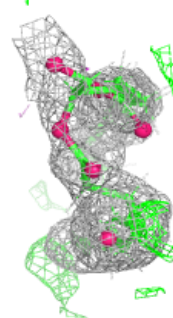
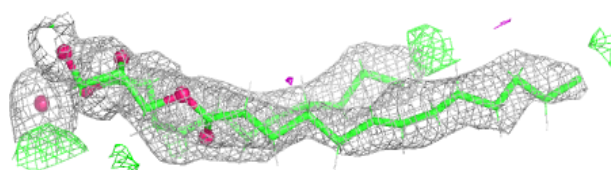
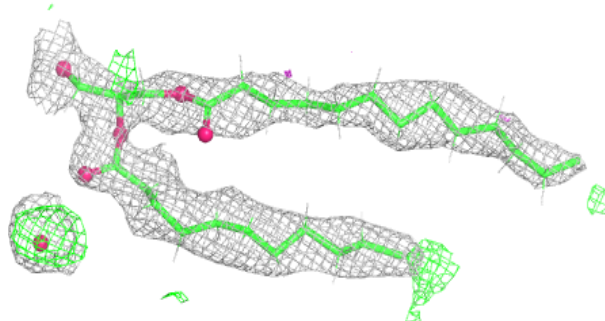
**Electron density around STE B 622:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

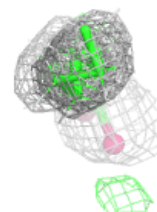
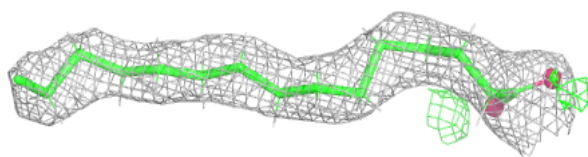
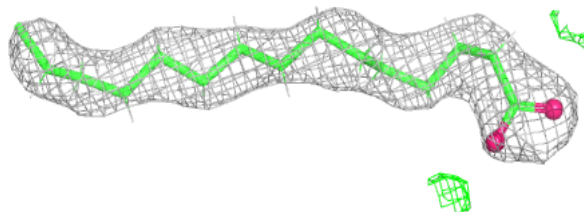


Electron density around LMG D 412:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

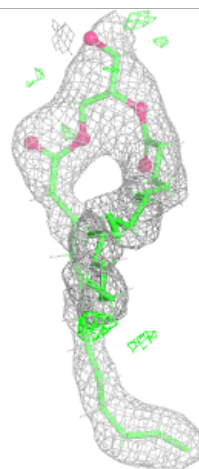
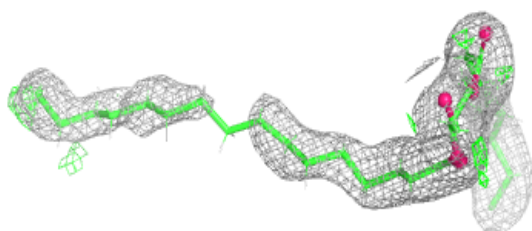
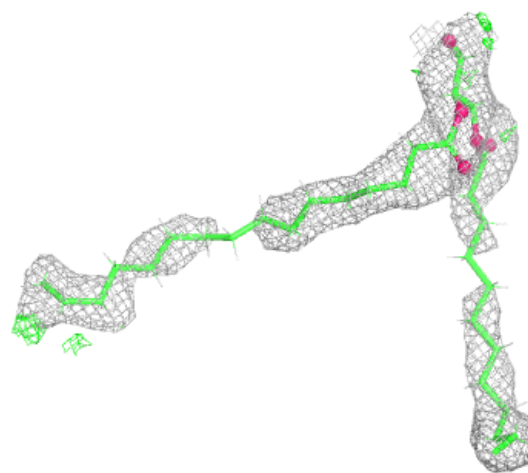
**Electron density around STE d 411:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



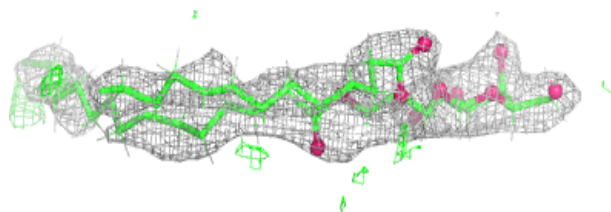
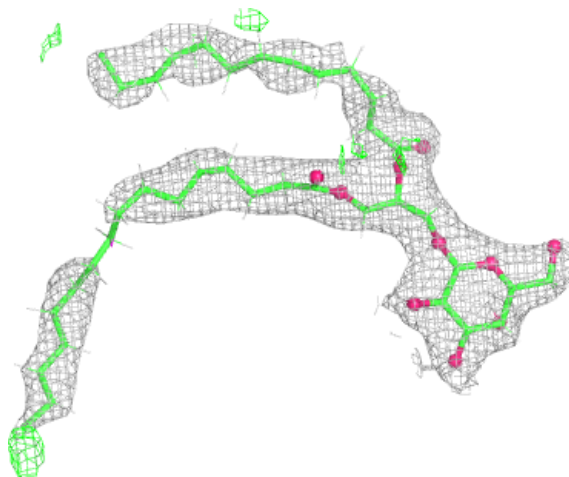
Electron density around SQD t 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



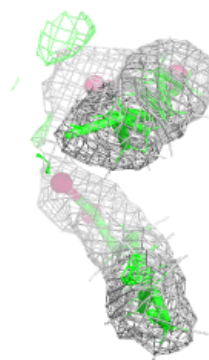
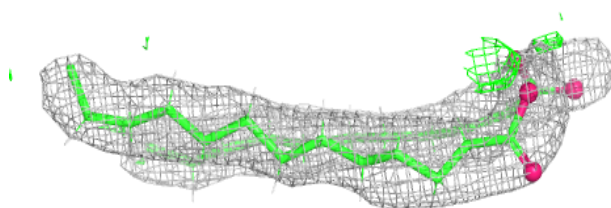
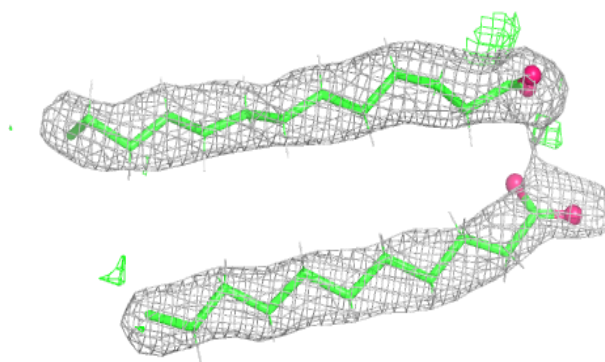
Electron density around LMG Y 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

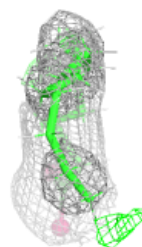
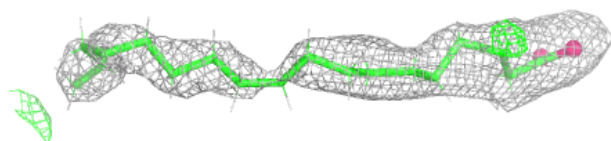
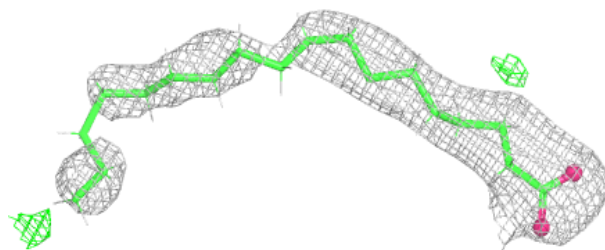


Electron density around LMG B 620:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

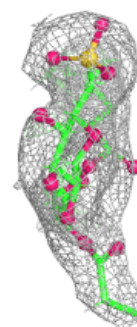
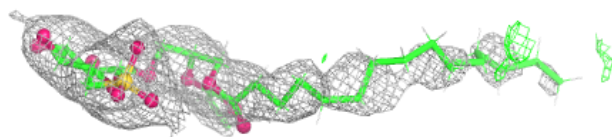
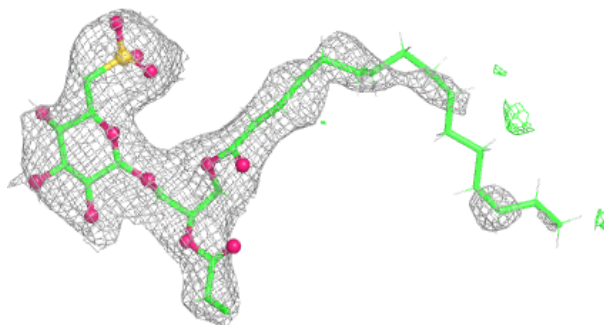
**Electron density around STE x 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

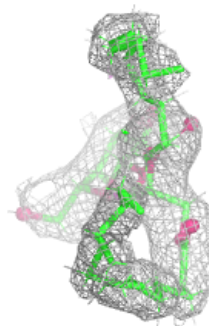
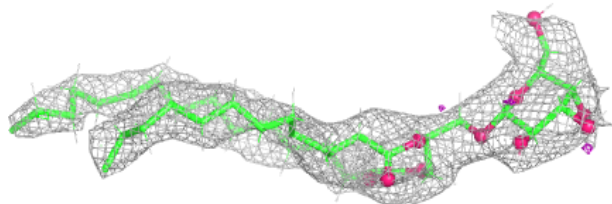
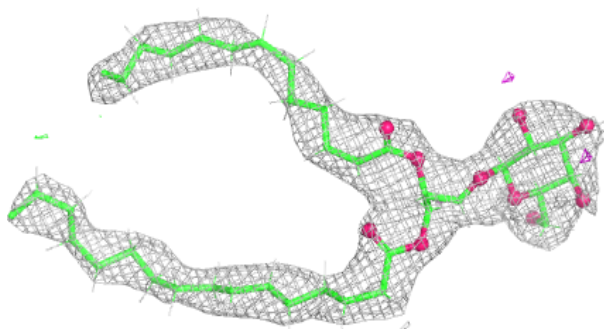


Electron density around SQD f 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

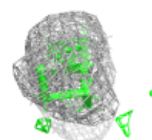
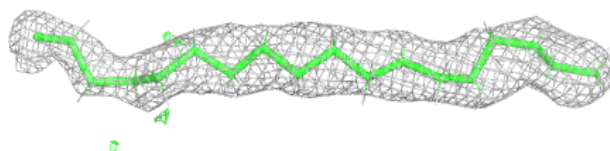
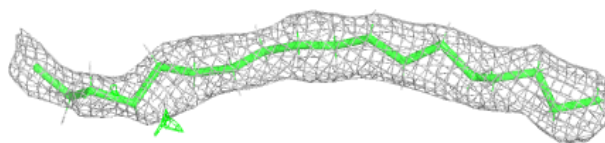
**Electron density around LMG A 409:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

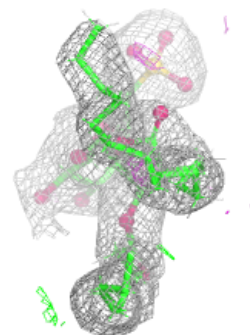
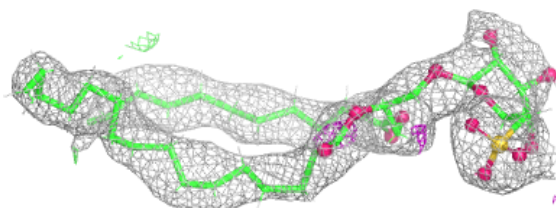
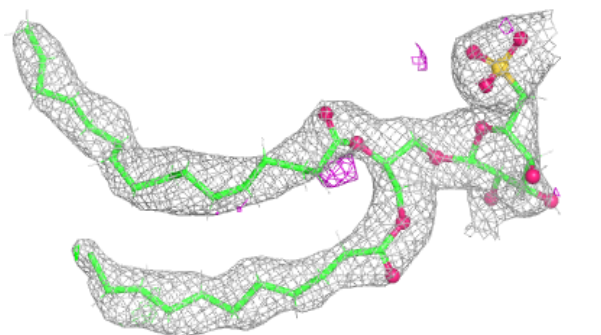


Electron density around STE M 104:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

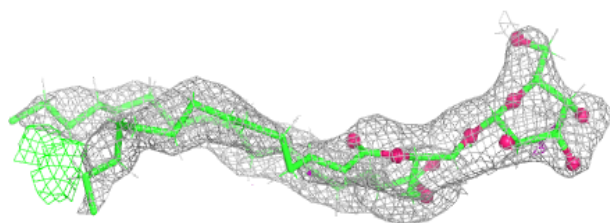
**Electron density around SQD L 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

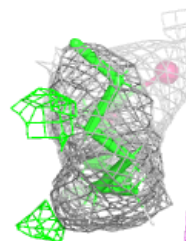
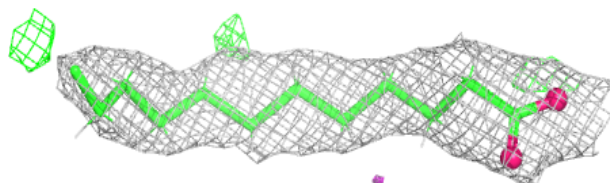
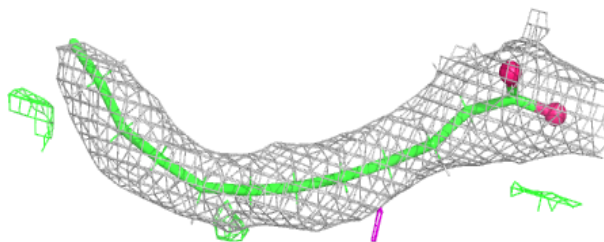


Electron density around LMG c 521:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

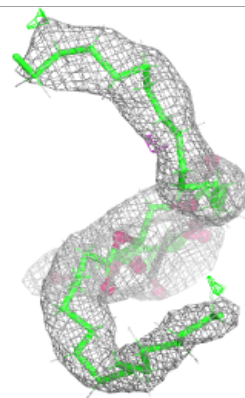
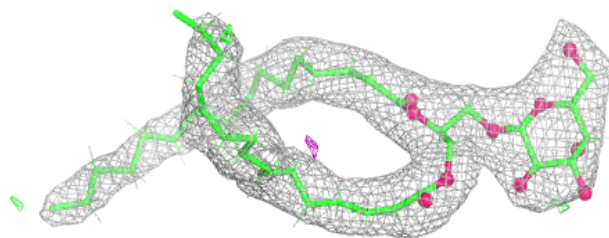
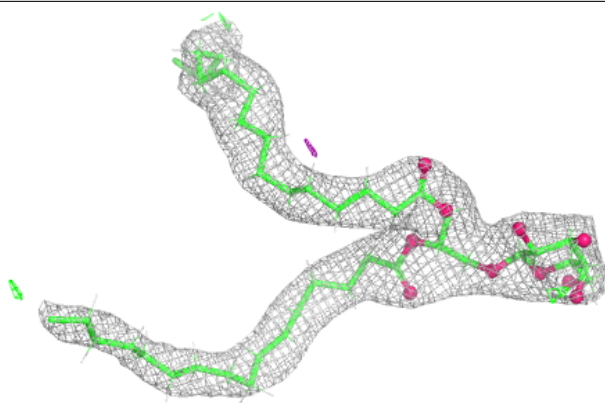
**Electron density around STE t 103:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

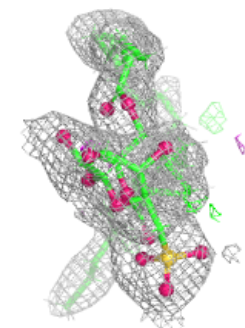
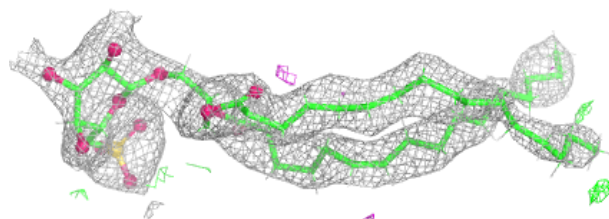
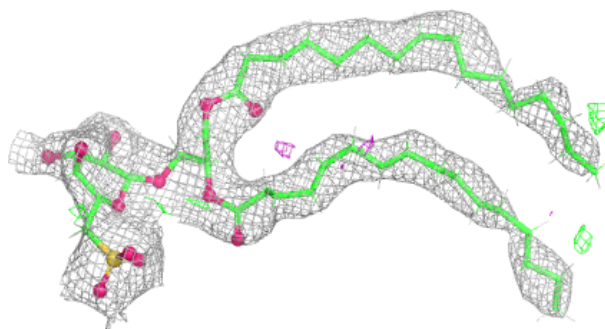


Electron density around LMG M 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

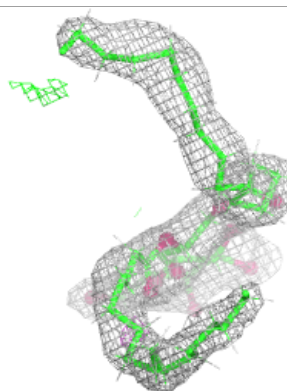
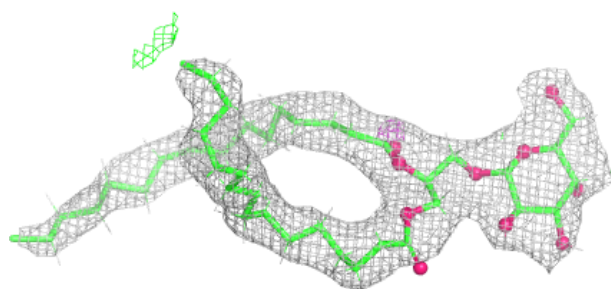
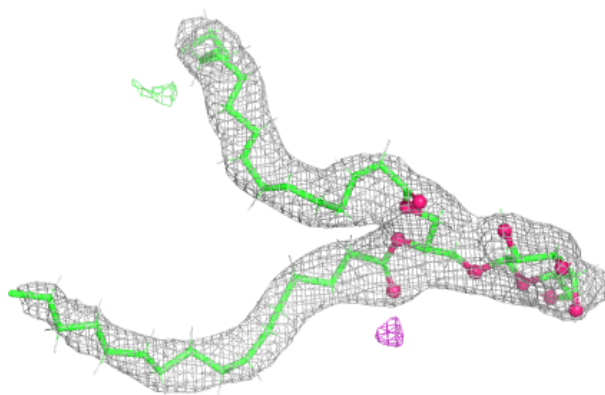
**Electron density around SQD B 621:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

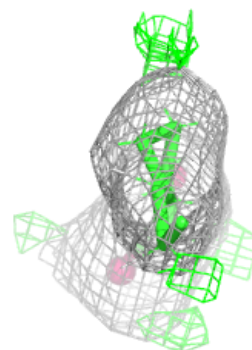
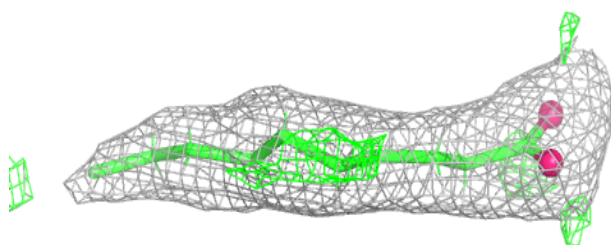
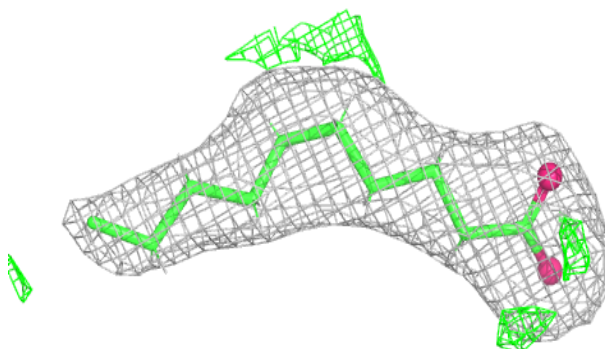


Electron density around LMG m 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

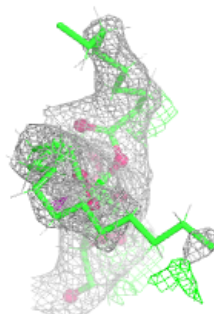
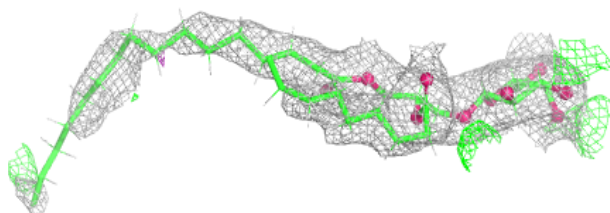
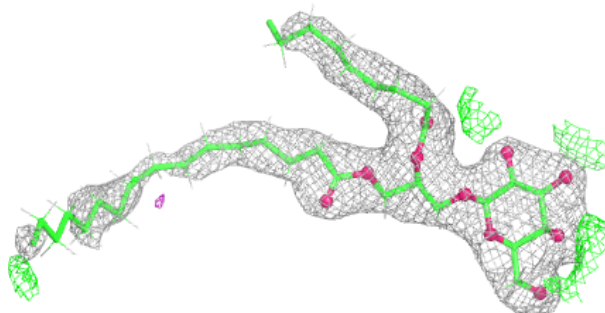
**Electron density around STE C 521:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

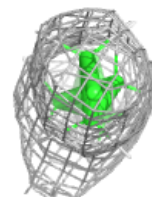
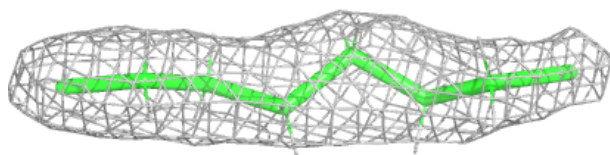
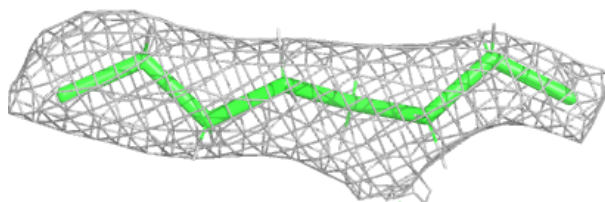


Electron density around LMG d 410:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

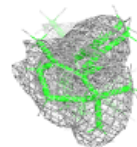
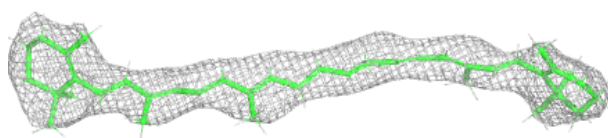
**Electron density around STE Z 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

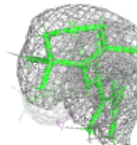
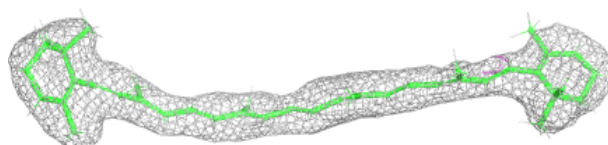
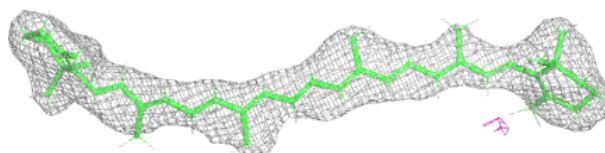


Electron density around BCR k 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

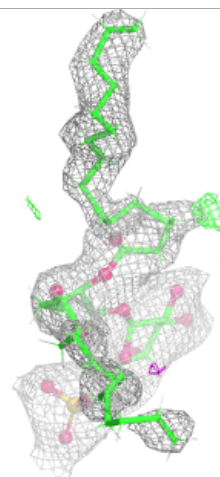
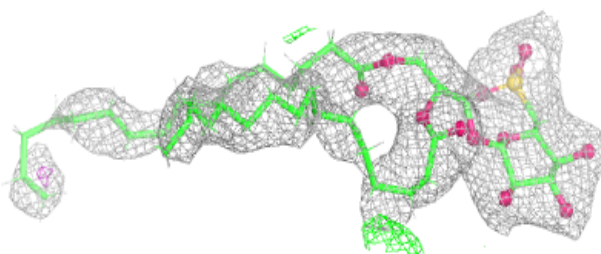
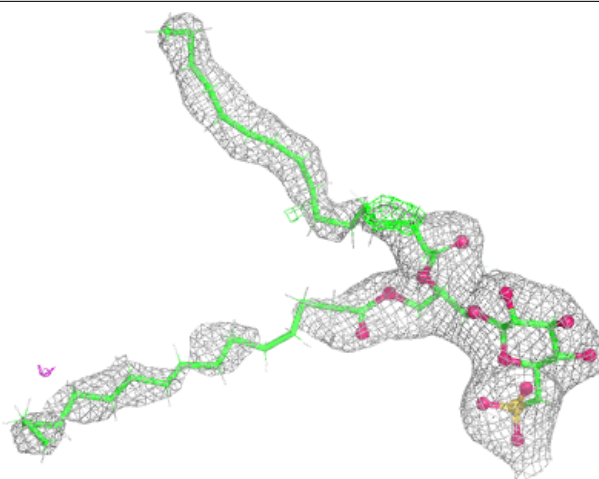
**Electron density around BCR x 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



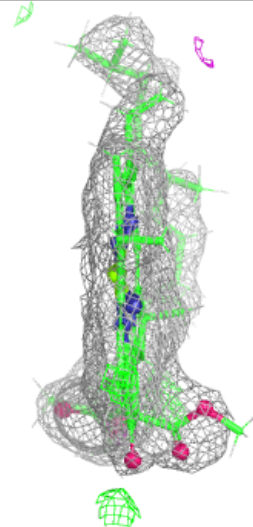
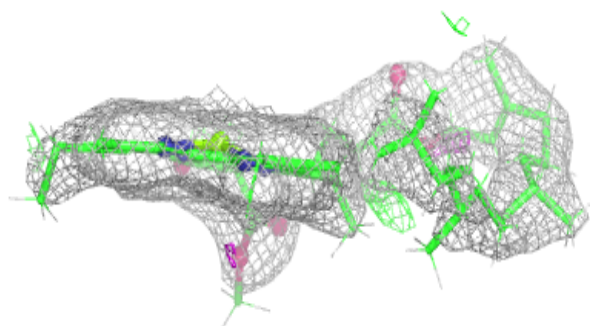
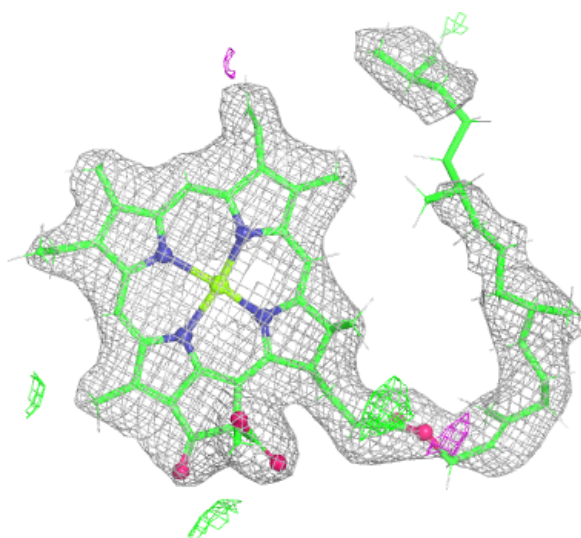
Electron density around SQD a 410:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



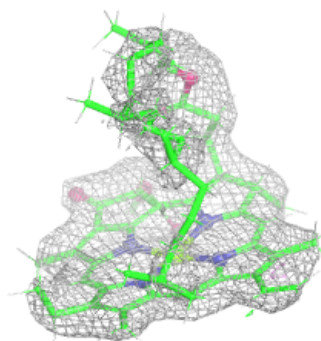
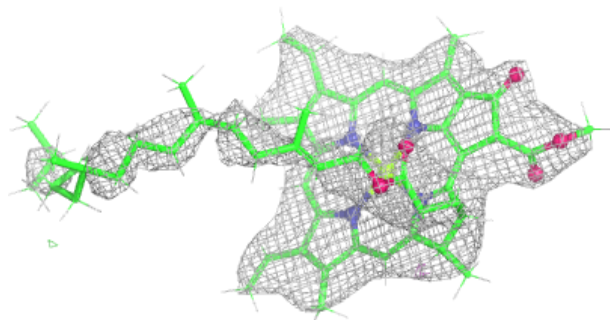
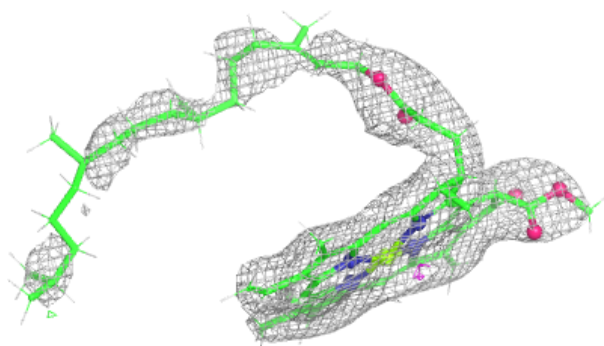
Electron density around CLA c 512:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

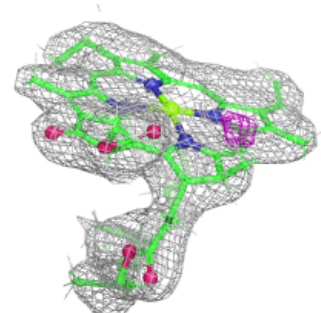
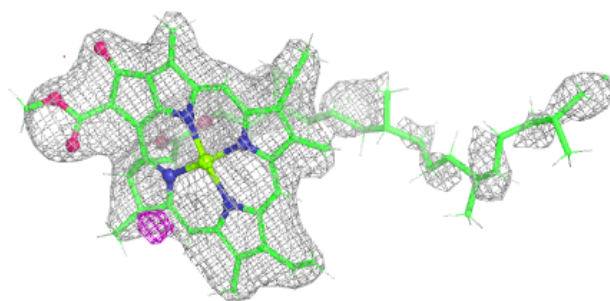
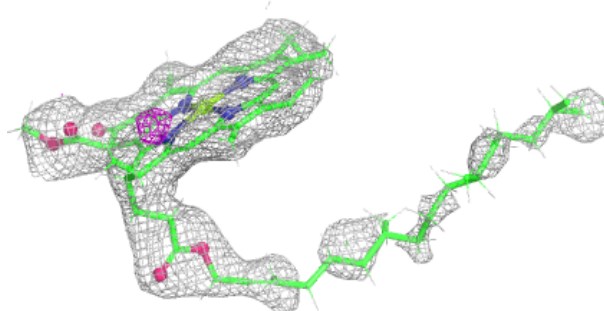


Electron density around CLA c 513:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

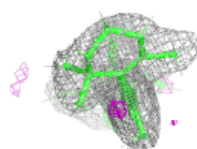
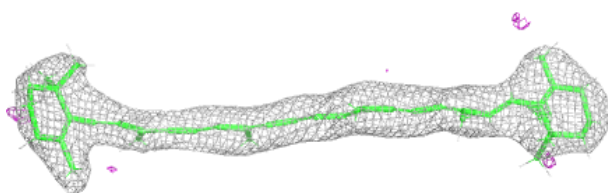
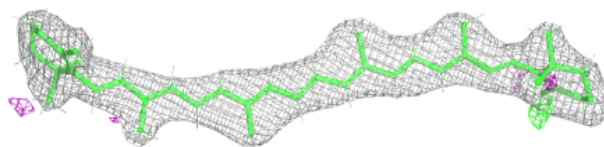
**Electron density around CLA C 513:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

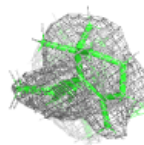
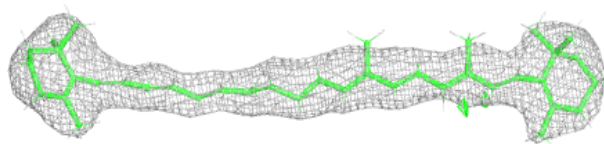


Electron density around BCR C 514:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

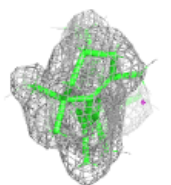
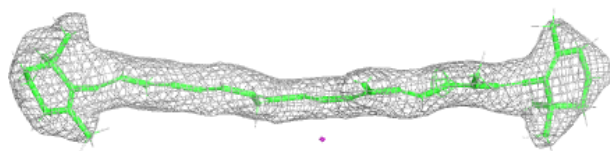
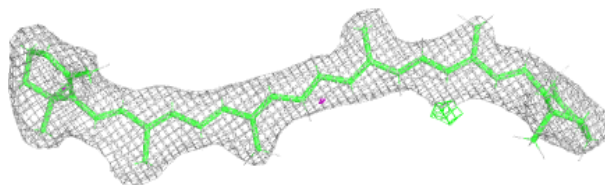
**Electron density around BCR K 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

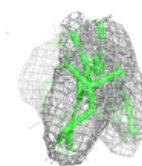
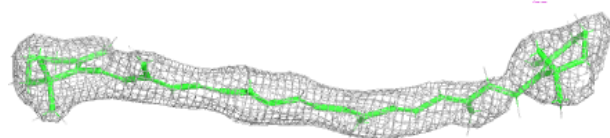
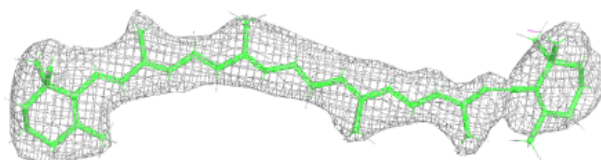


Electron density around BCR K 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

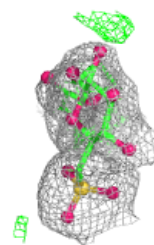
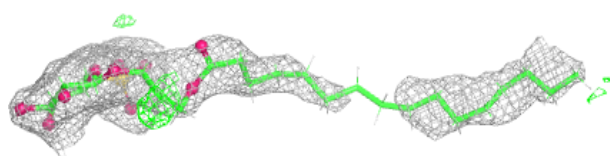
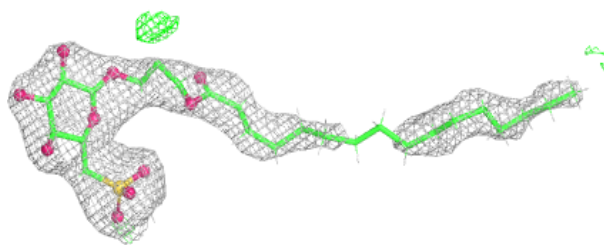
**Electron density around BCR d 406:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

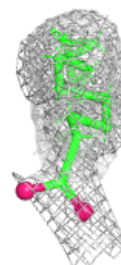
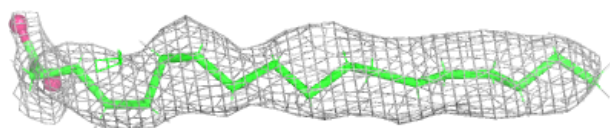
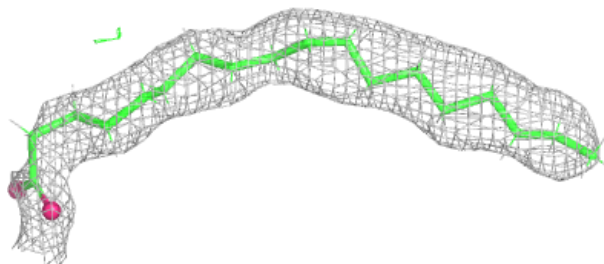


Electron density around SQD D 409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

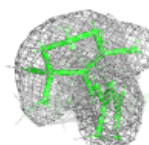
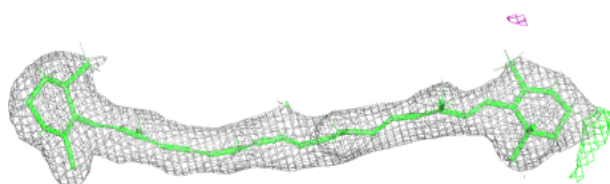
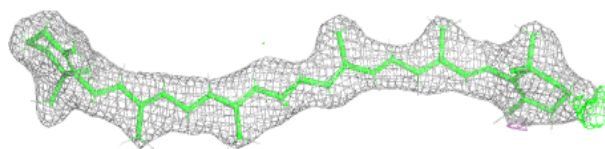
**Electron density around STE X 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

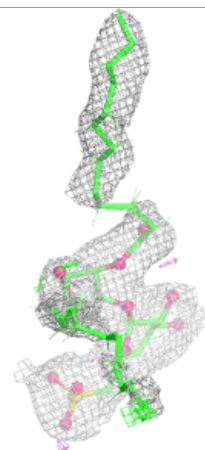
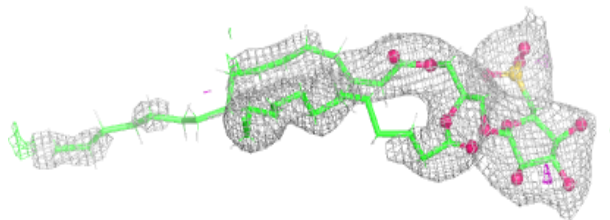
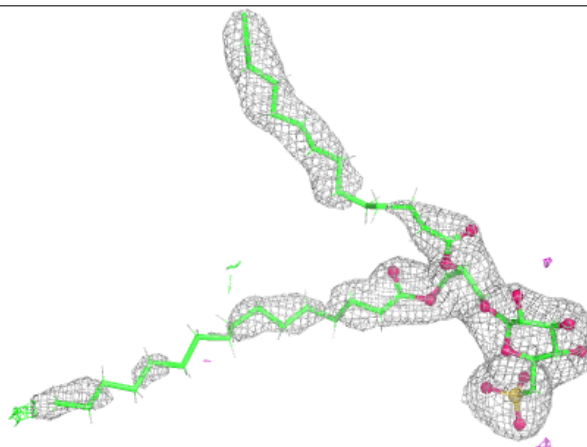


Electron density around BCR H 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

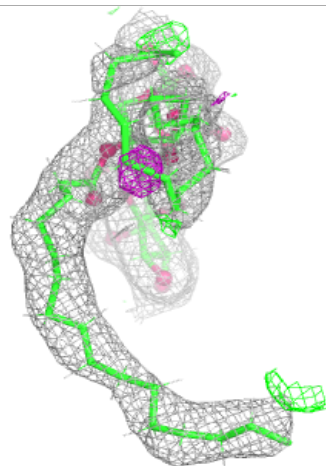
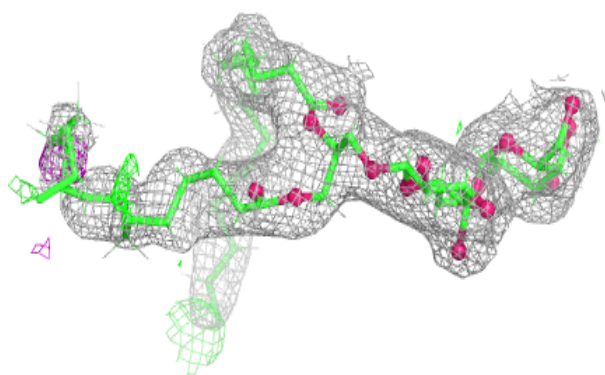
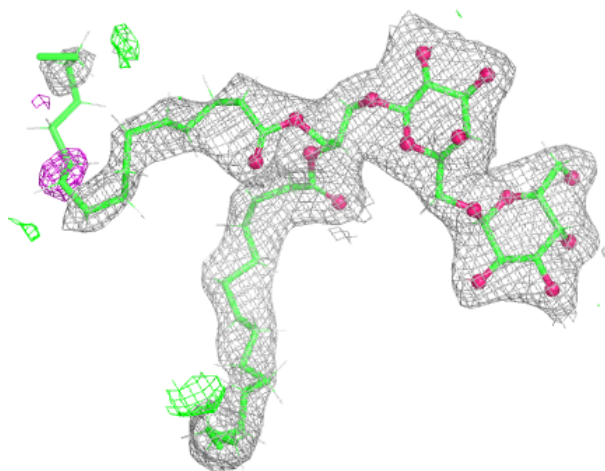
**Electron density around SQD A 410:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



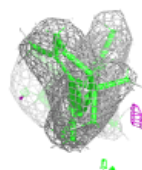
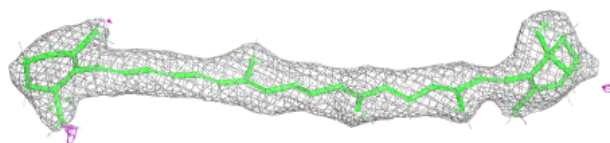
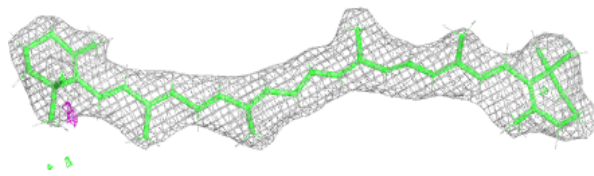
Electron density around DGD C 517:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

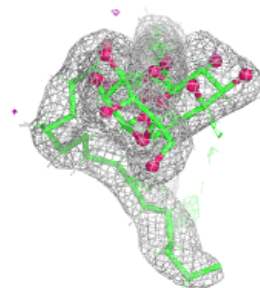
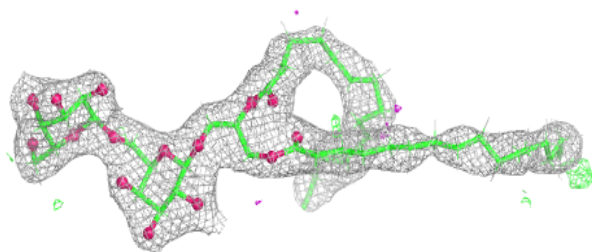
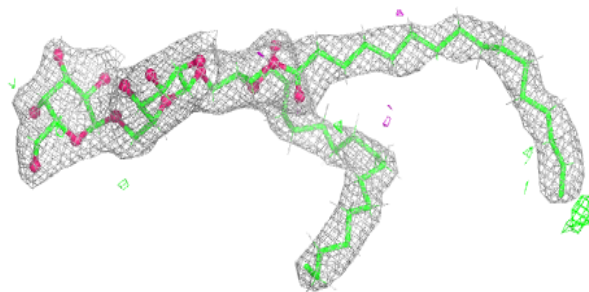


Electron density around BCR b 619:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

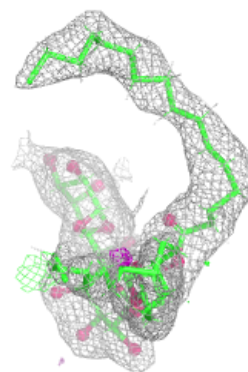
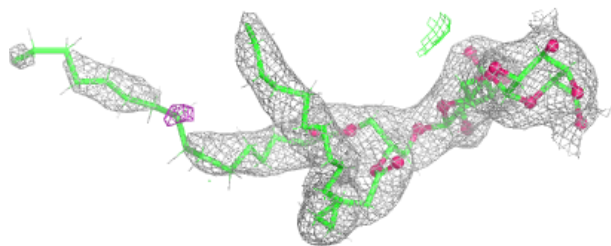
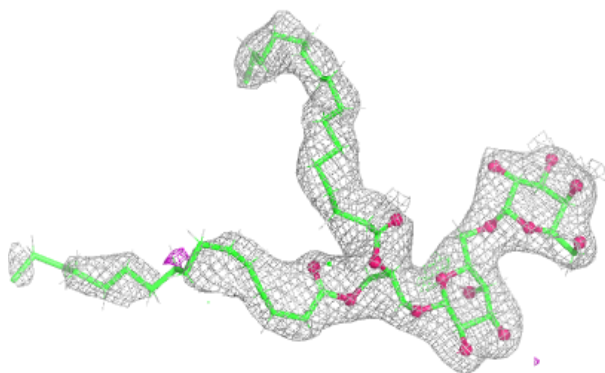
**Electron density around DGD H 103:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

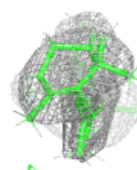
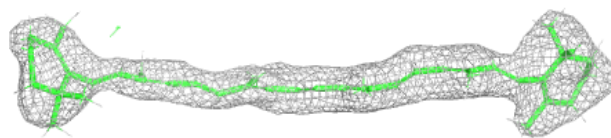
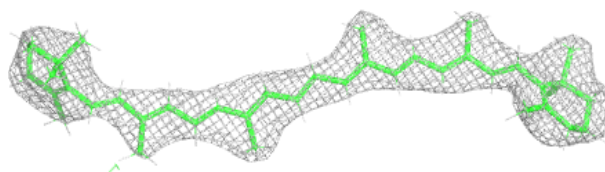


Electron density around DGD c 516:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

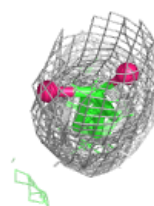
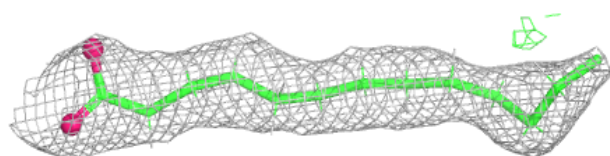
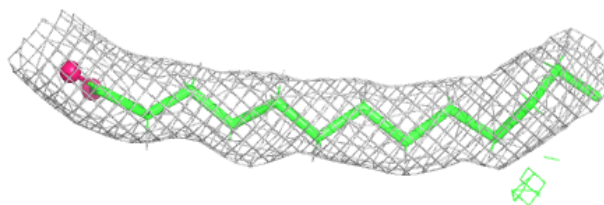
**Electron density around BCR k 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

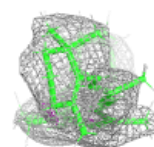
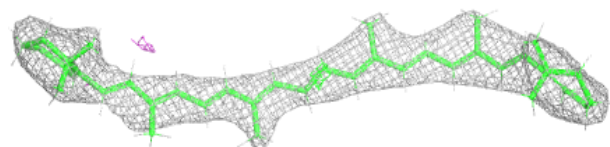
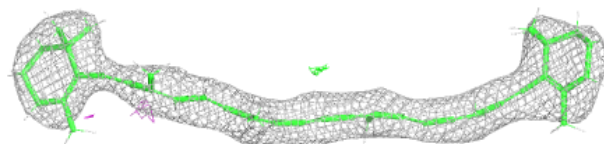


Electron density around STE M 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

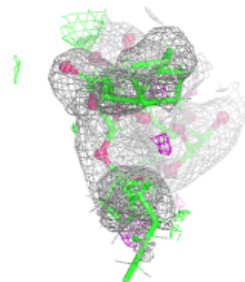
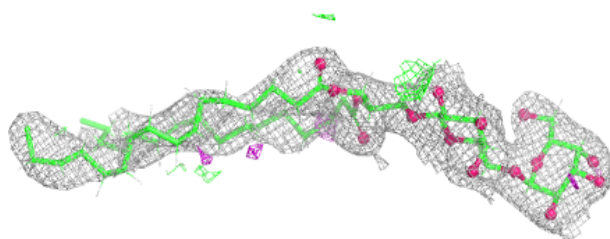
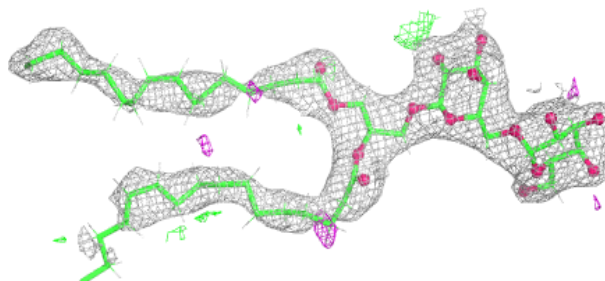
**Electron density around BCR k 103:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

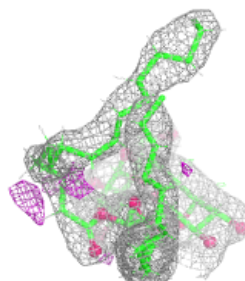
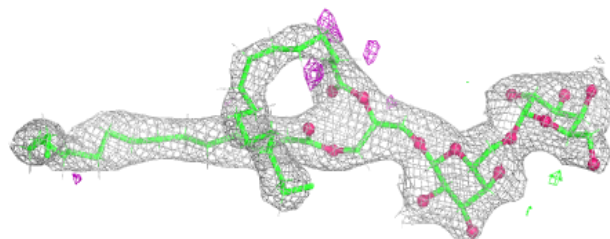
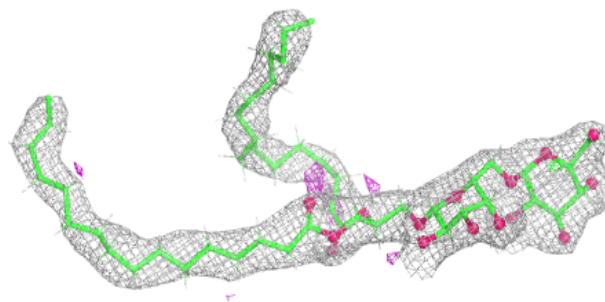


Electron density around DGD c 517:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

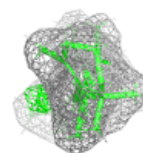
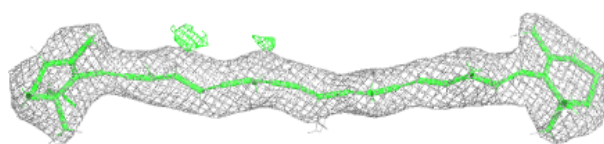
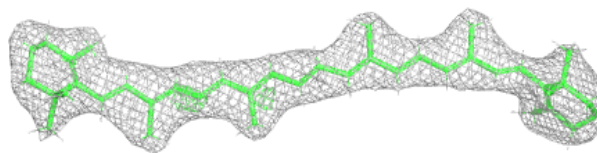
**Electron density around DGD h 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

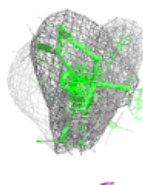
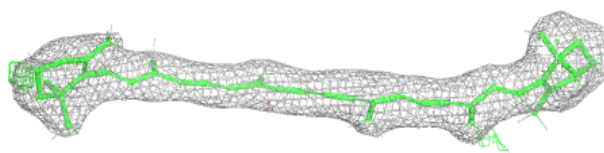
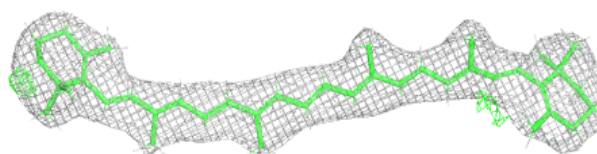


Electron density around BCR B 617:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

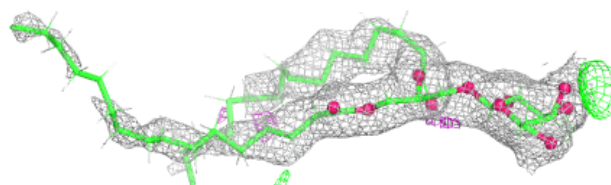
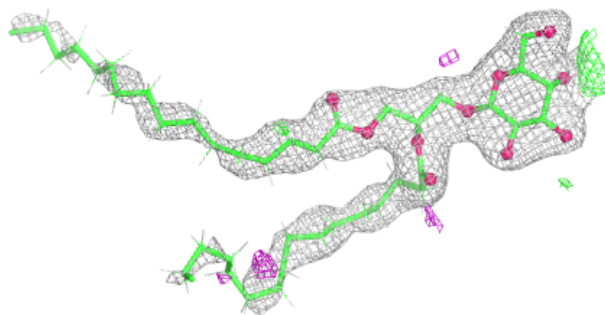
**Electron density around BCR B 618:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

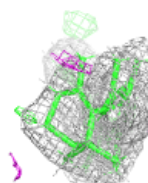
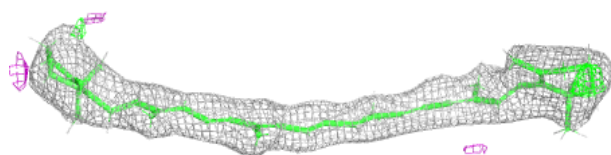
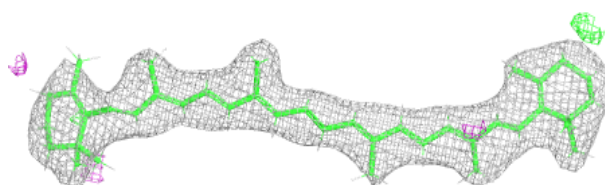


Electron density around LMG D 408:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

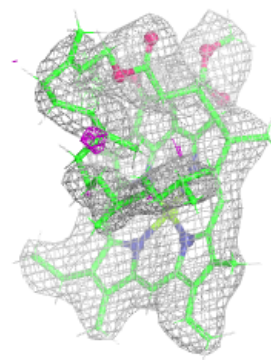
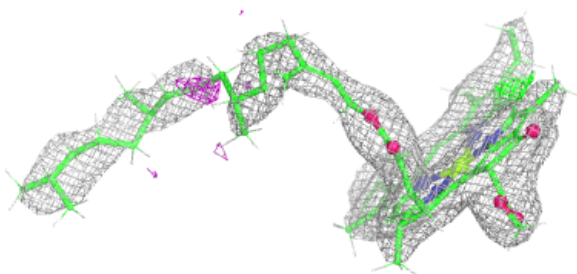
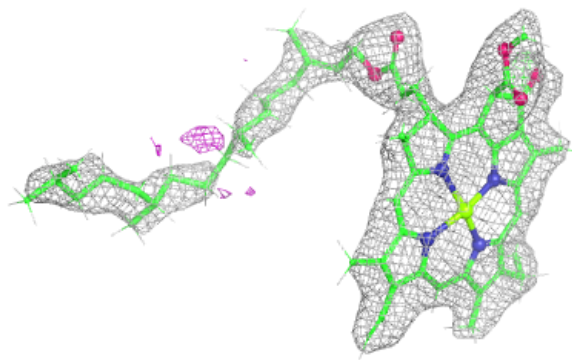
**Electron density around BCR D 406:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

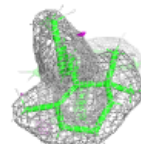
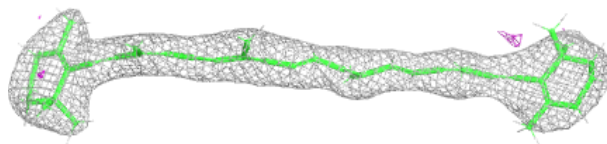
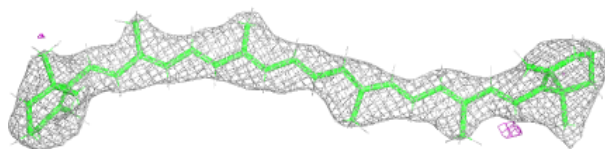


Electron density around CLA c 511:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

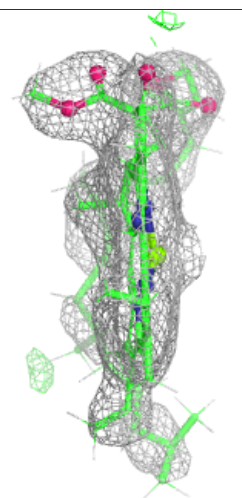
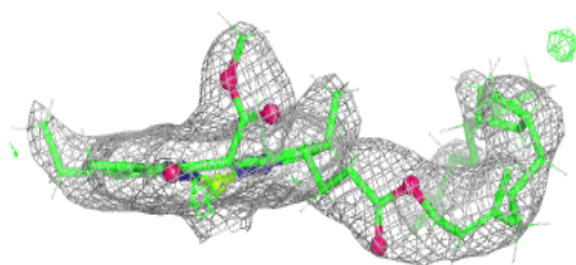
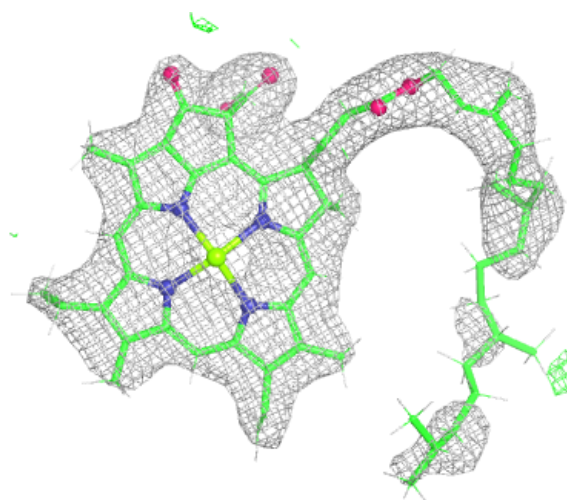
**Electron density around BCR c 514:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



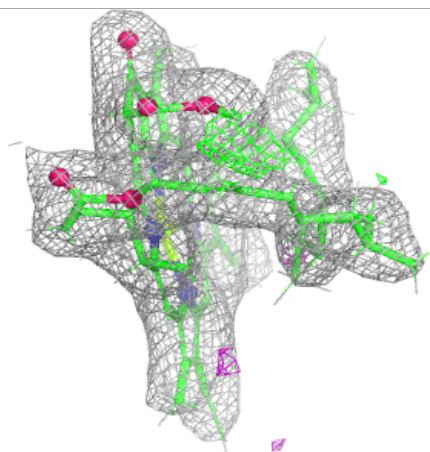
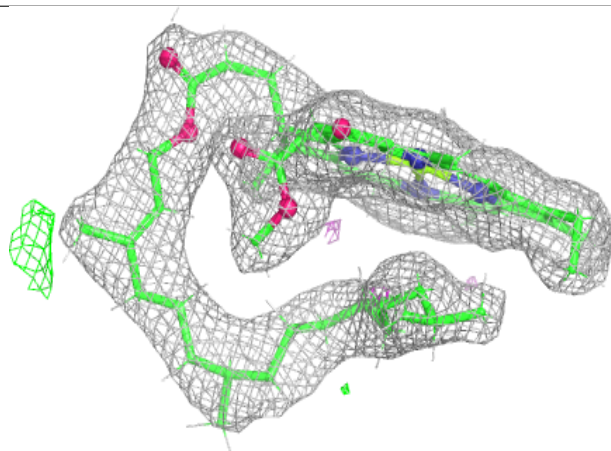
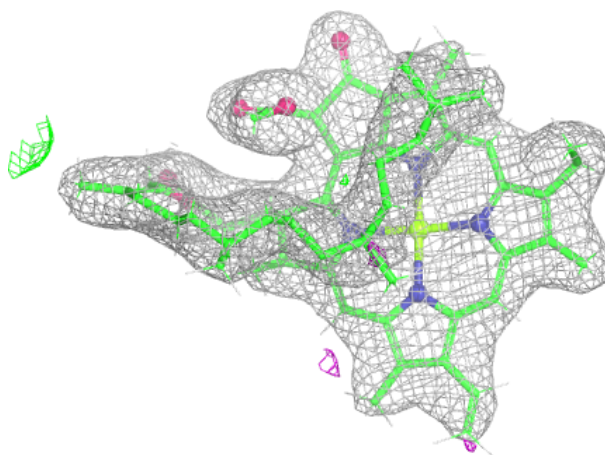
Electron density around CLA C 512:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



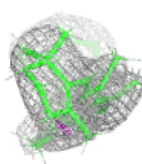
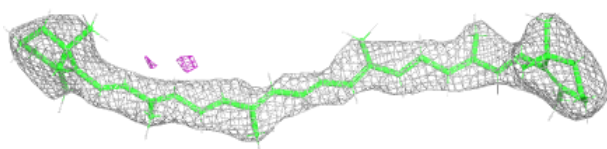
Electron density around CLA C 510:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

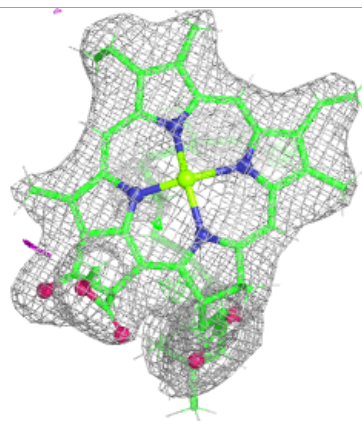
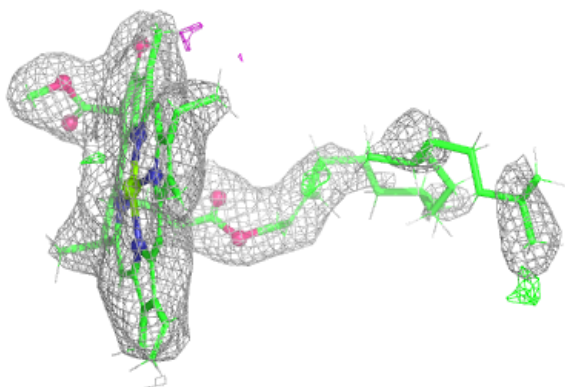
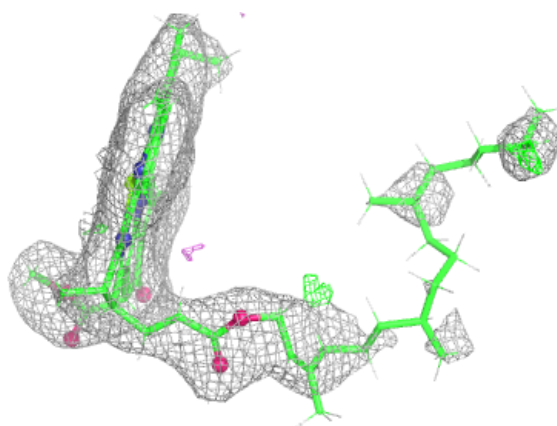


Electron density around BCR C 515:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

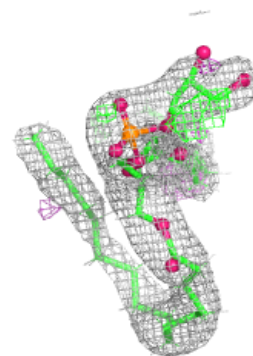
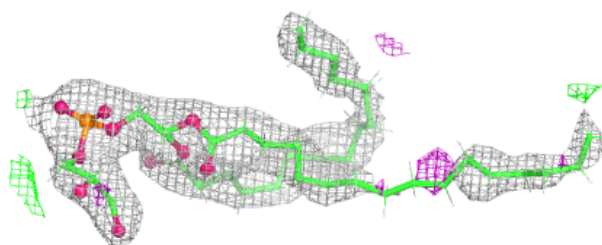
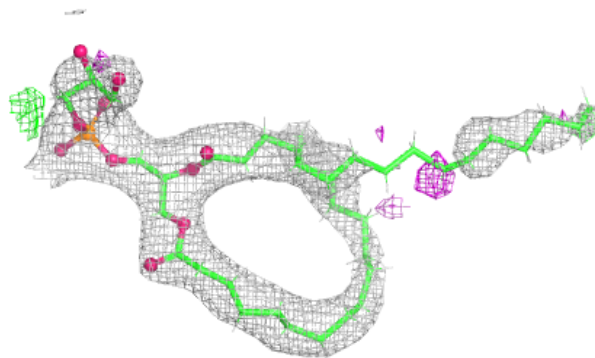
**Electron density around CLA c 506:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

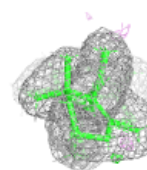
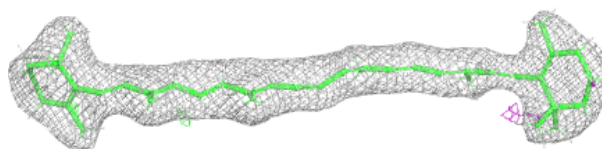
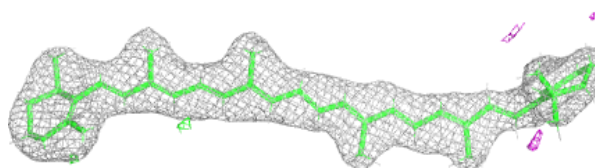


Electron density around LHG b 623:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

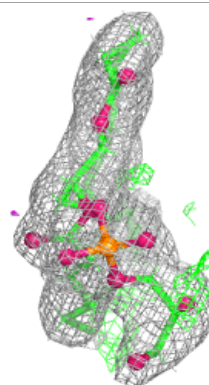
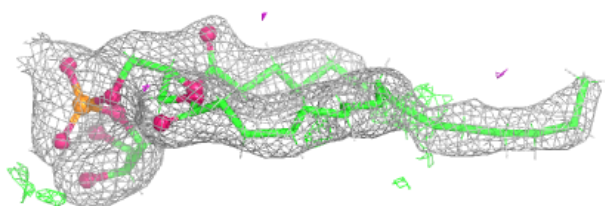
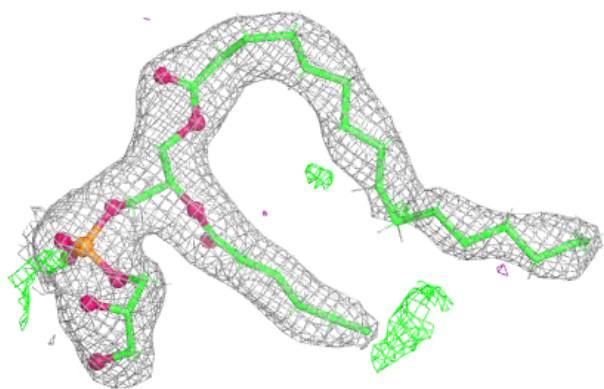
**Electron density around BCR I 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

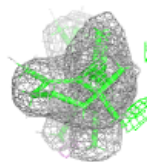
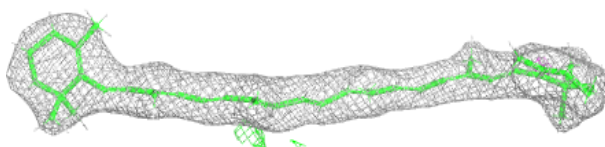
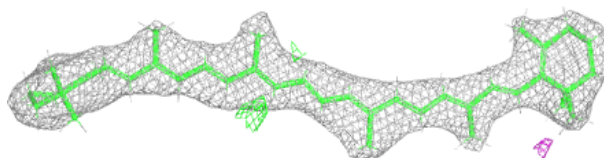


Electron density around LHG d 409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

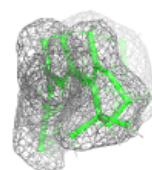
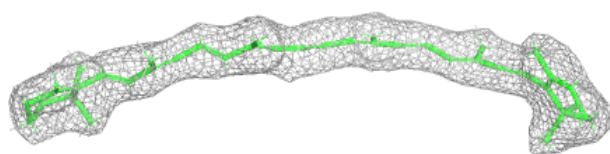
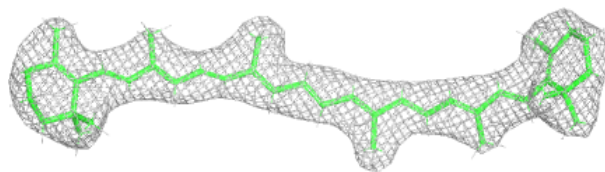
**Electron density around BCR B 616:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

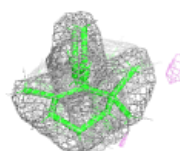
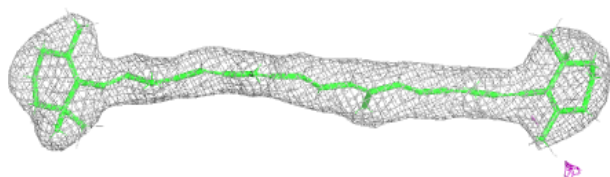
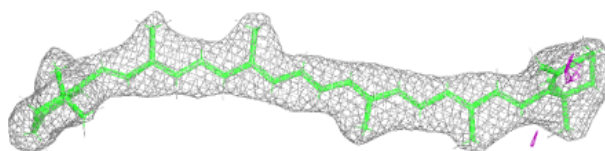


Electron density around BCR T 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

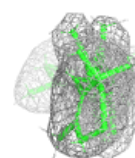
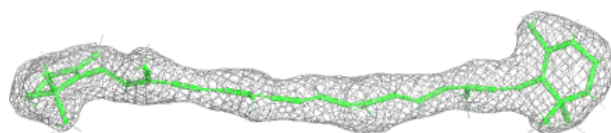
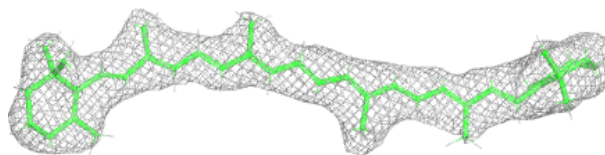
**Electron density around BCR a 406:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

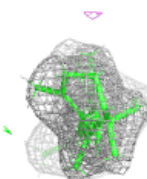
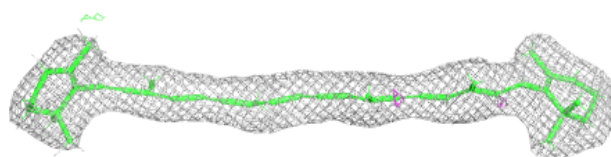
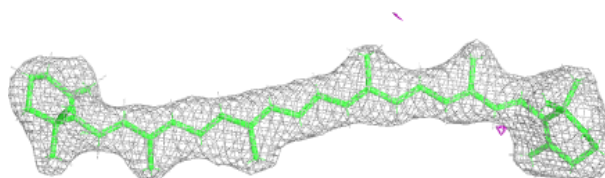


Electron density around BCR b 617:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

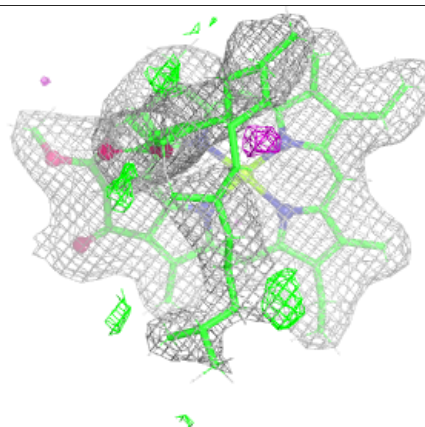
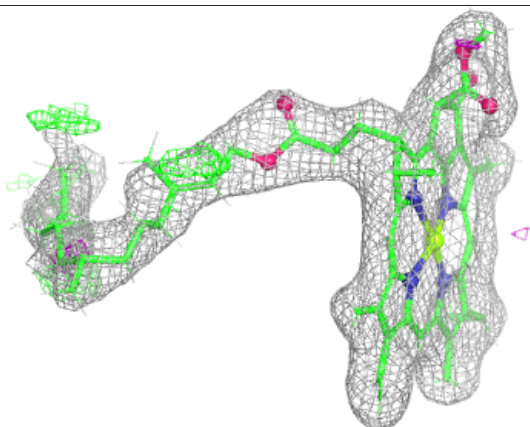
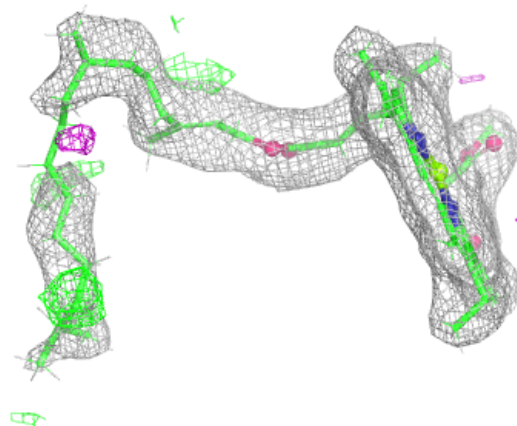
**Electron density around BCR b 618:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



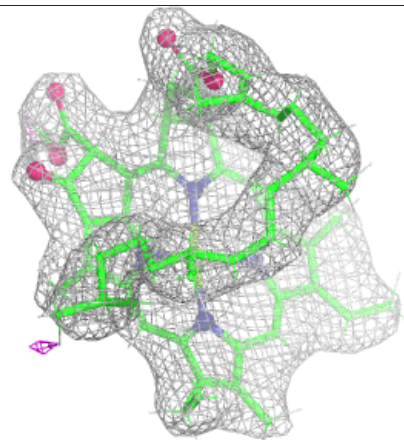
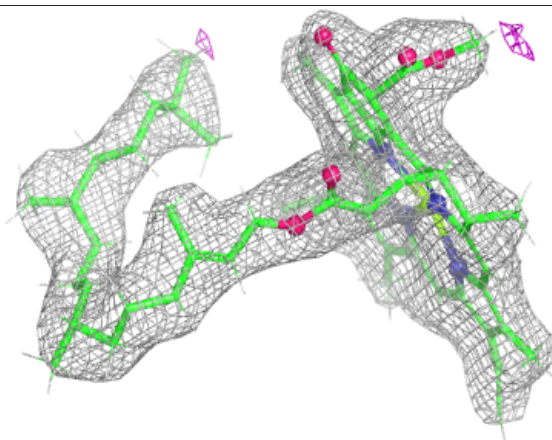
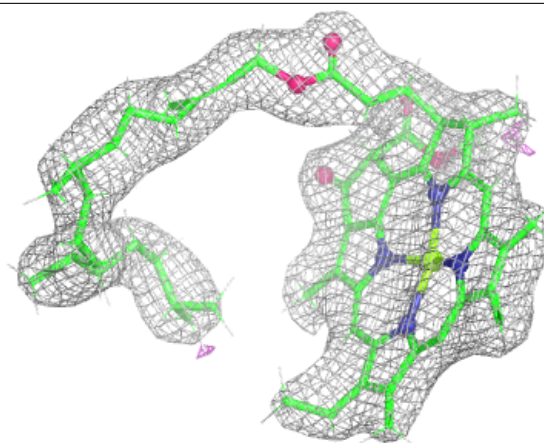
Electron density around CLA a 405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



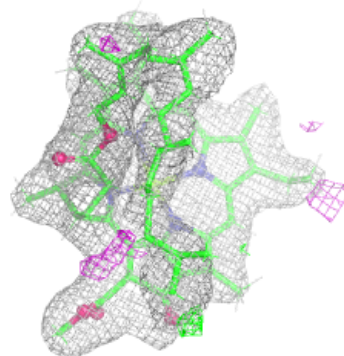
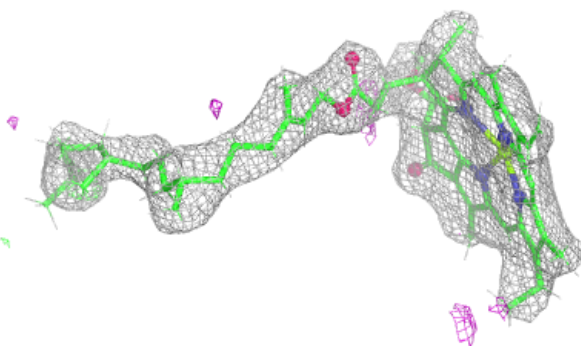
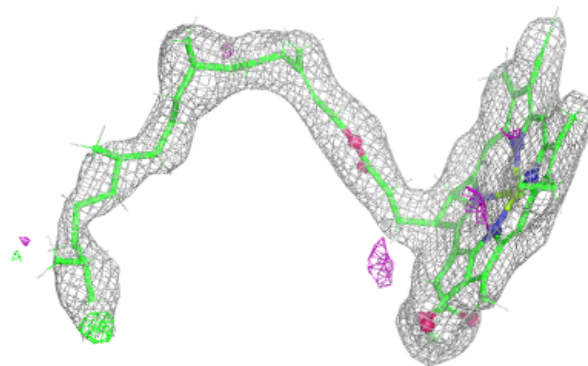
Electron density around CLA C 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

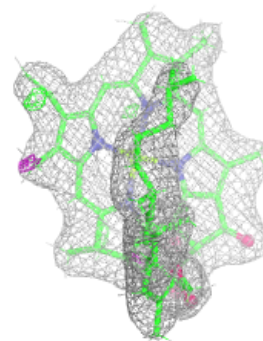
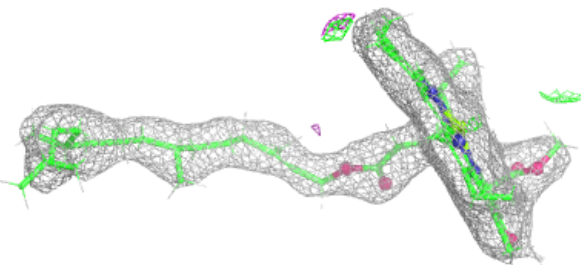
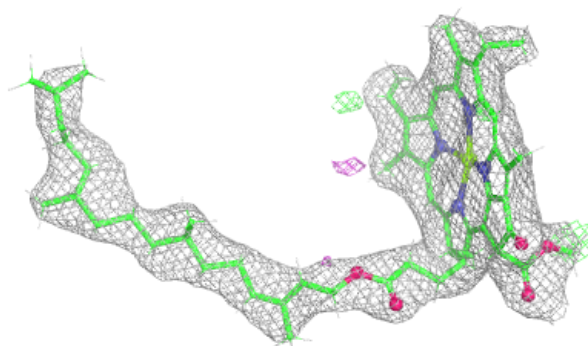


Electron density around CLA b 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

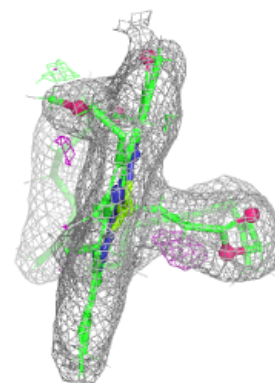
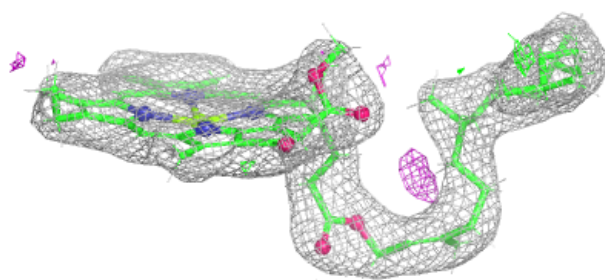
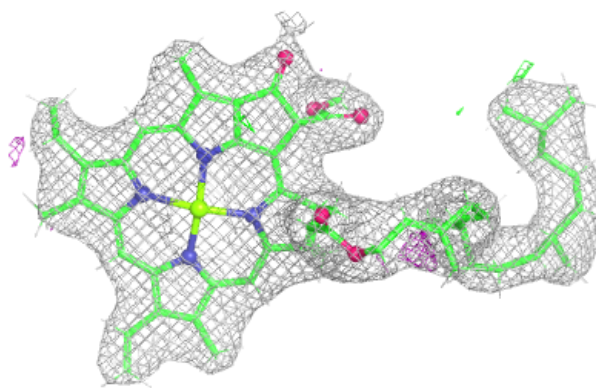
**Electron density around CLA b 609:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



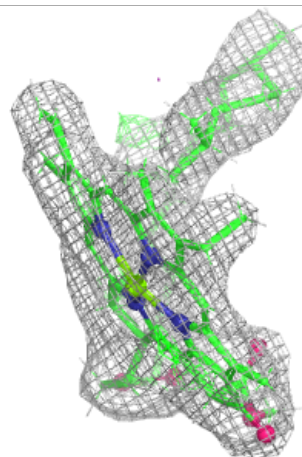
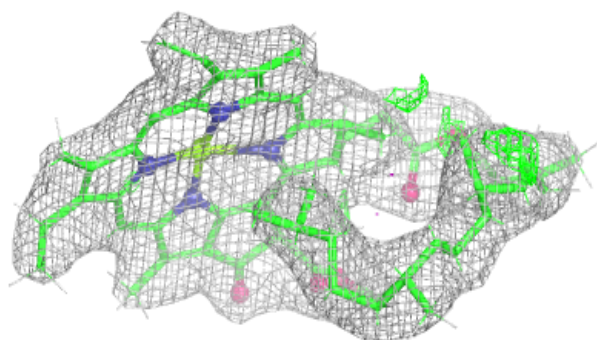
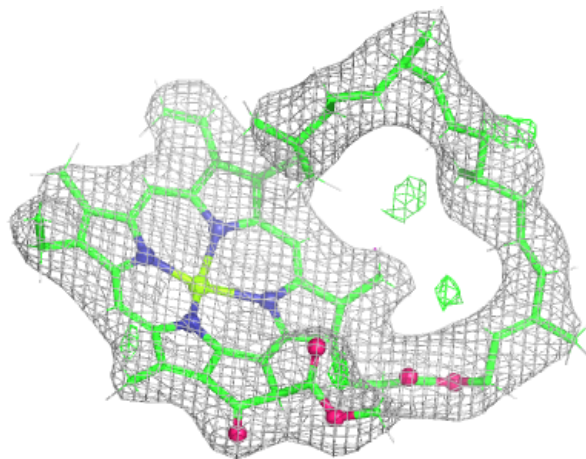
Electron density around CLA b 612:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



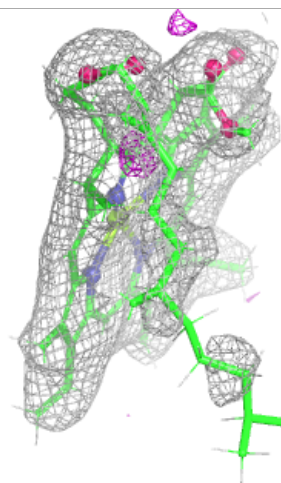
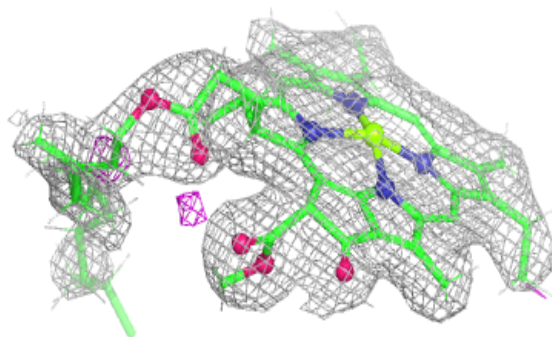
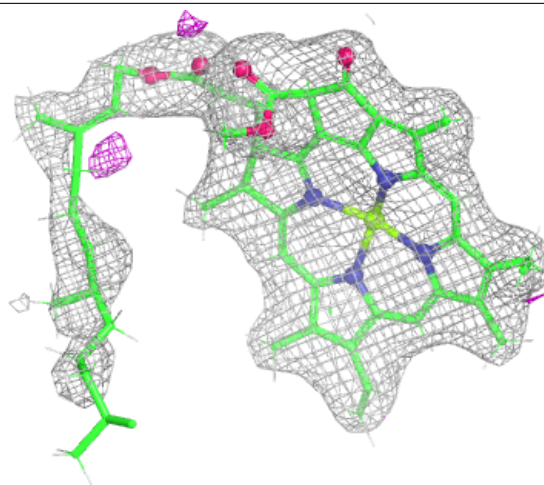
Electron density around CLA b 615:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



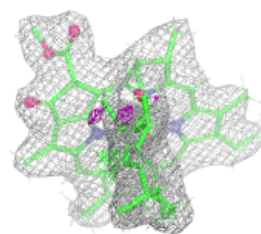
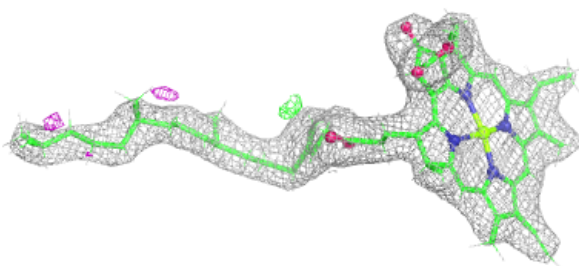
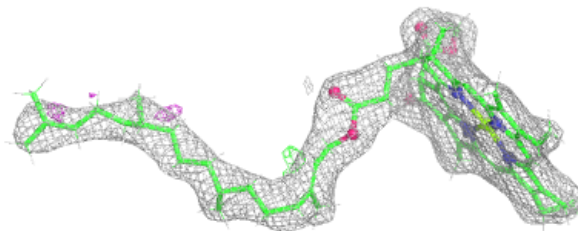
Electron density around CLA b 616:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



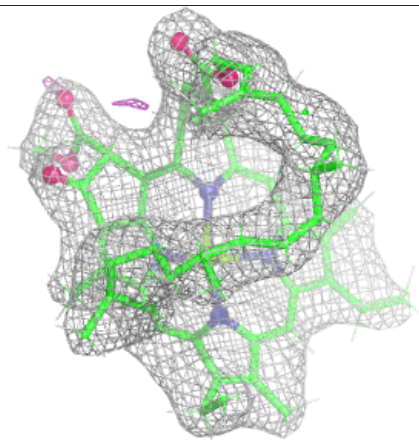
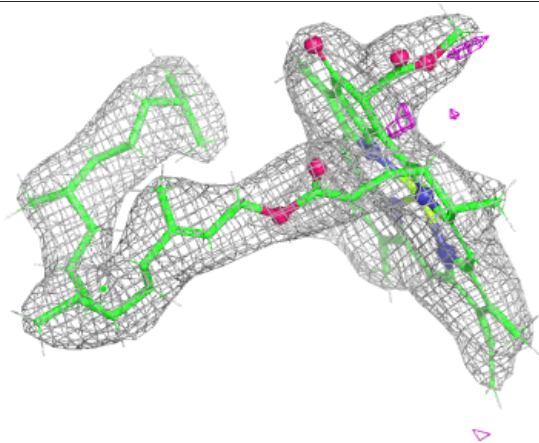
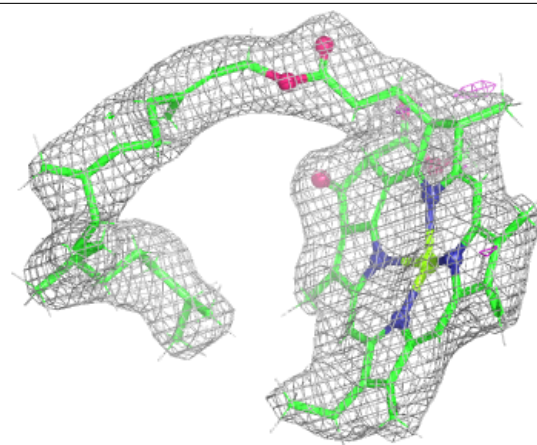
Electron density around CLA c 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



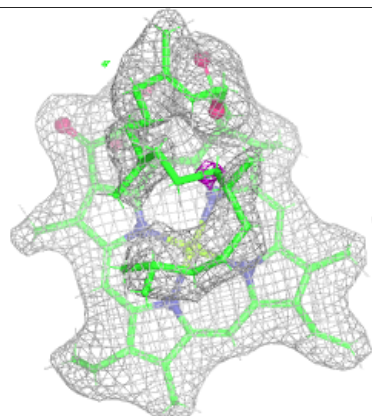
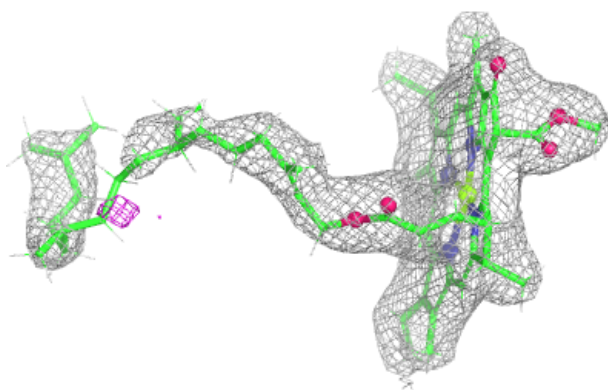
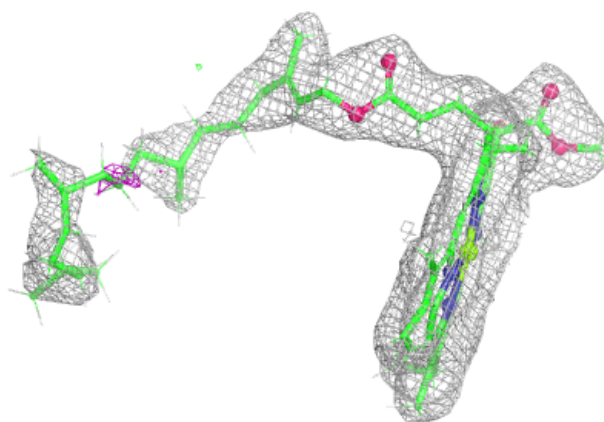
Electron density around CLA c 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

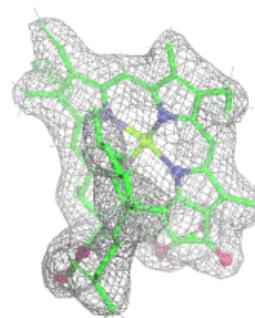
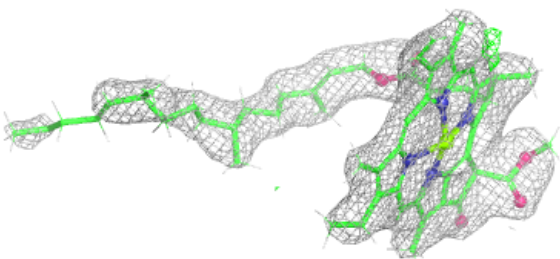
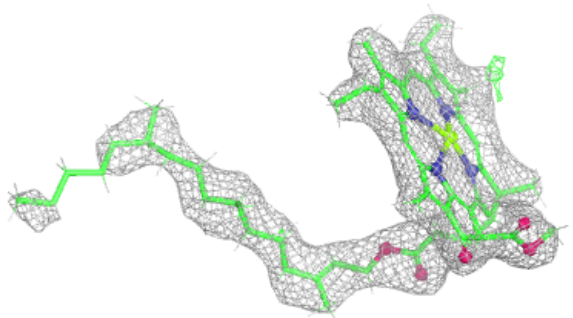


Electron density around CLA C 506:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

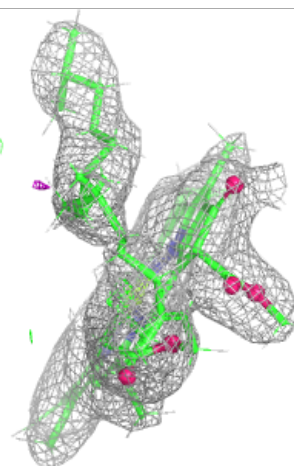
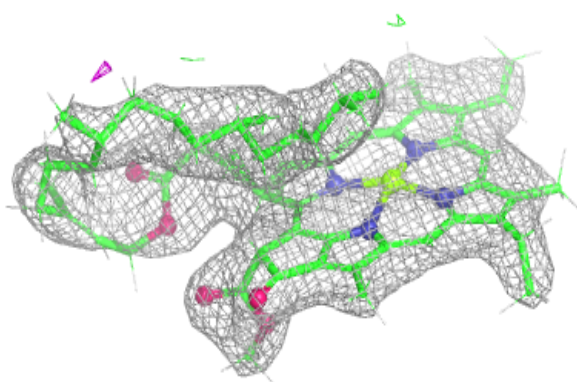
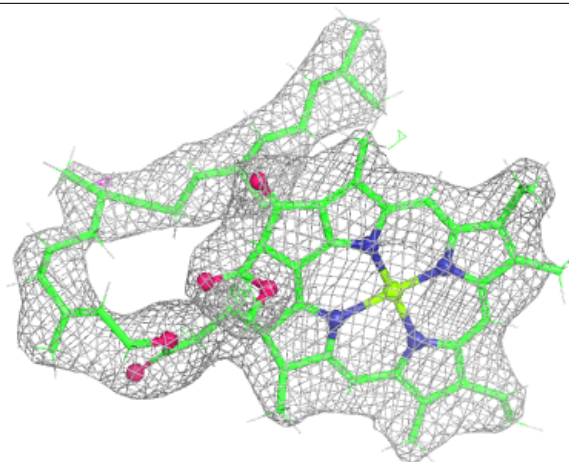
**Electron density around CLA c 508:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



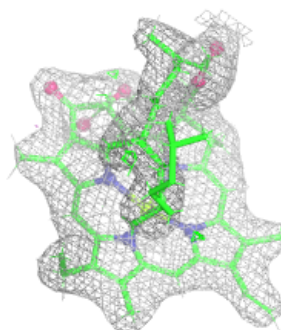
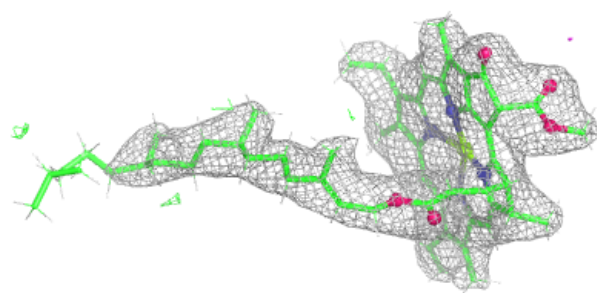
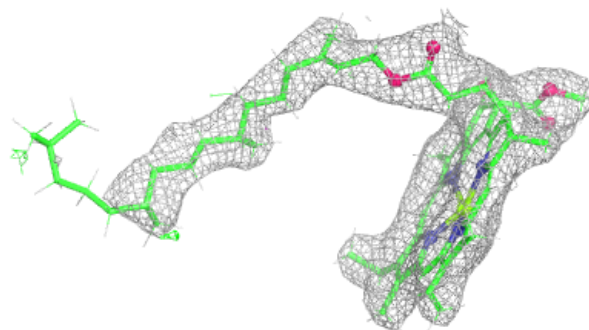
Electron density around CLA c 509:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



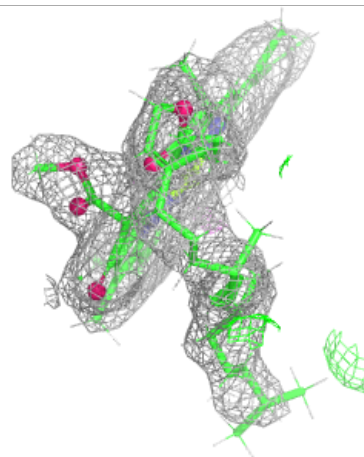
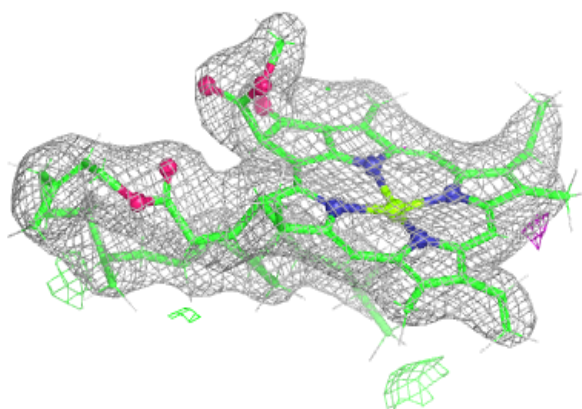
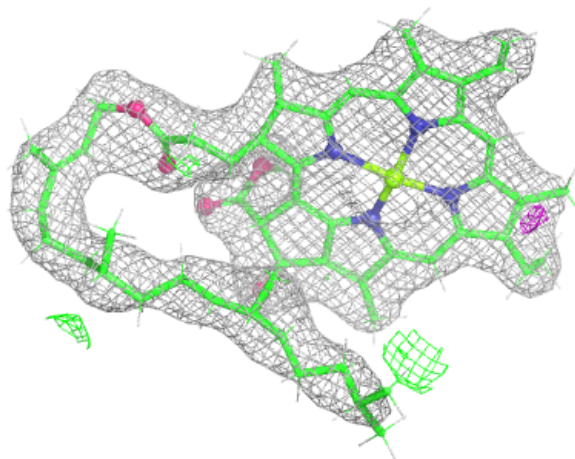
Electron density around CLA C 508:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



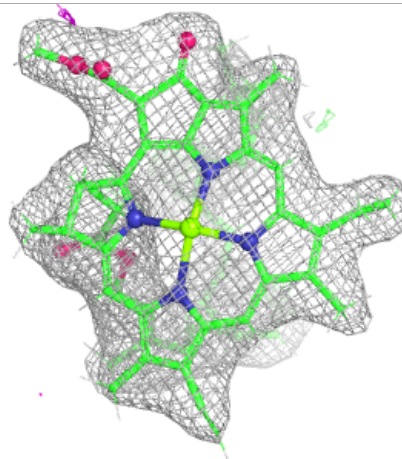
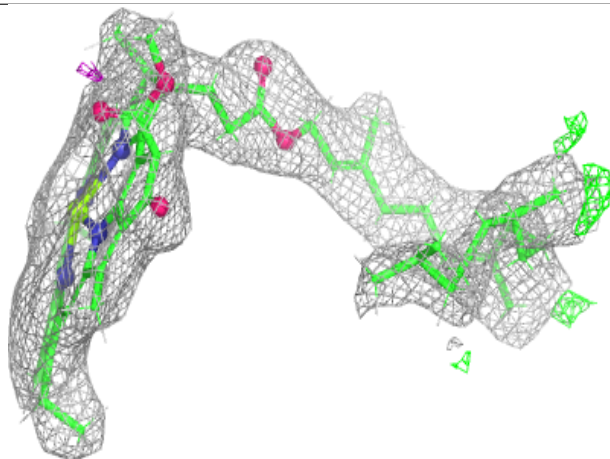
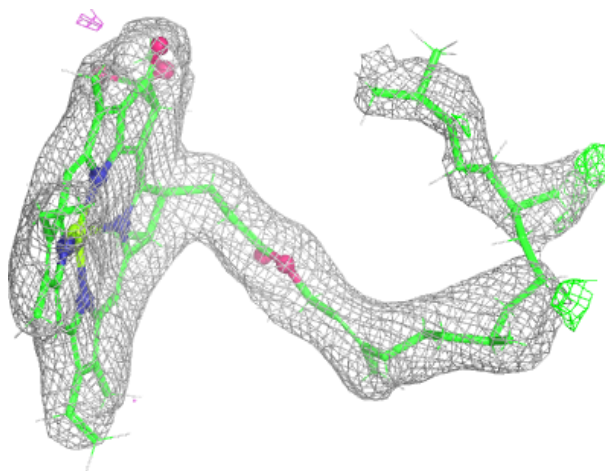
Electron density around CLA C 509:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



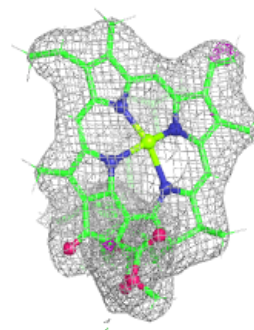
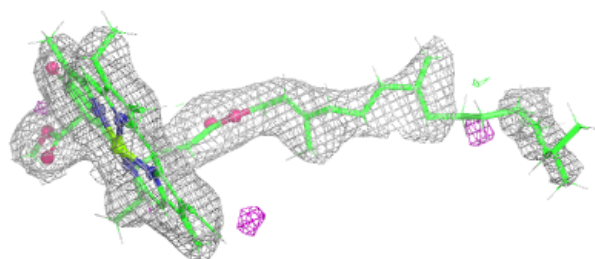
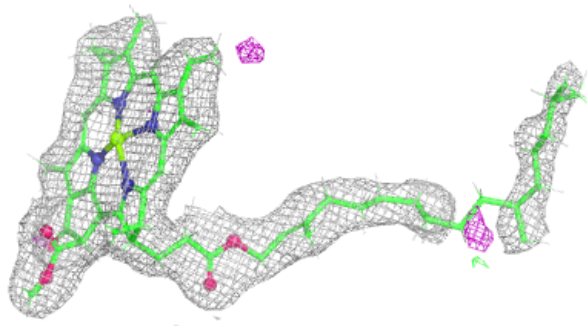
Electron density around CLA B 605:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



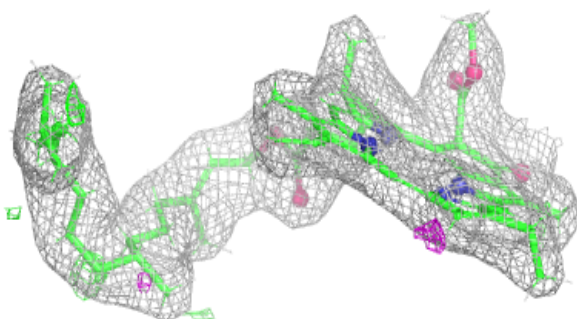
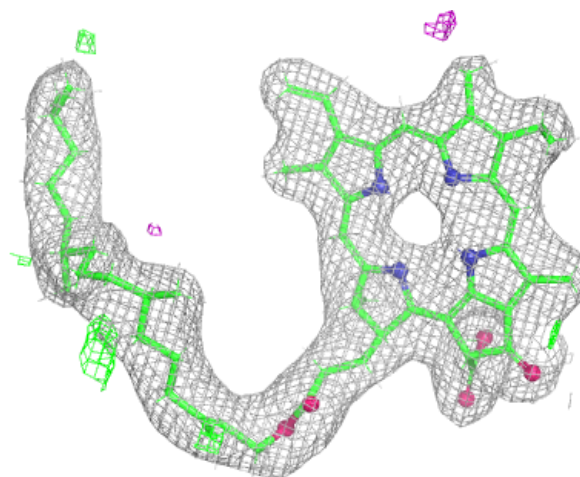
Electron density around CLA d 405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



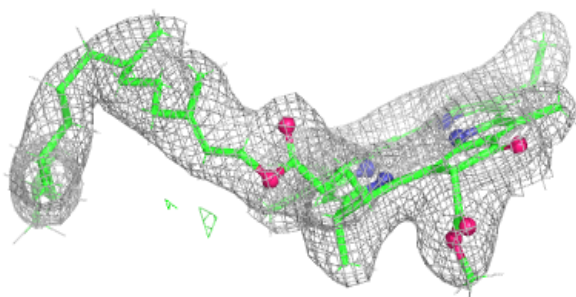
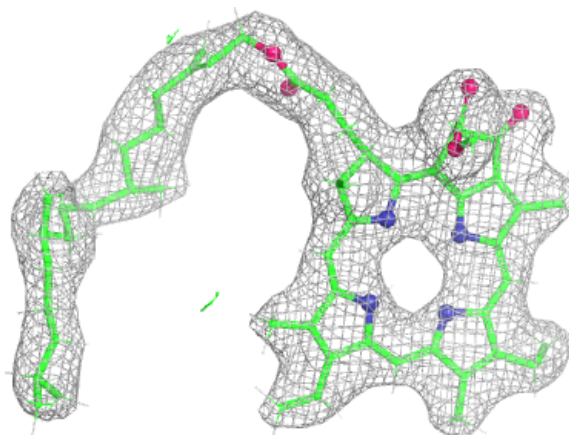
Electron density around PHO D 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



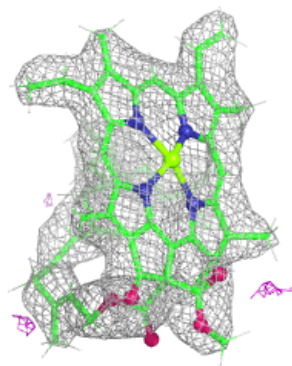
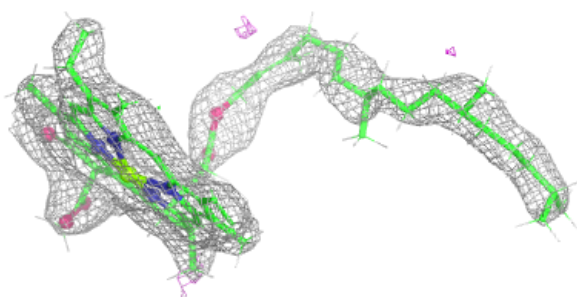
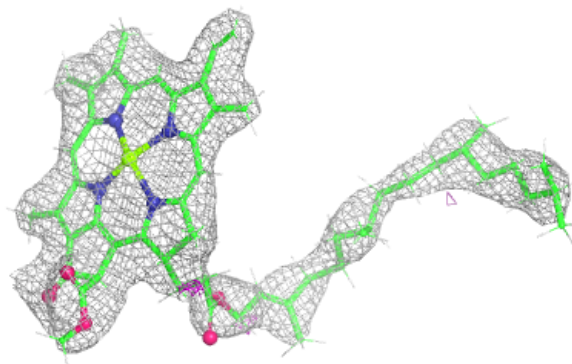
Electron density around PHO d 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

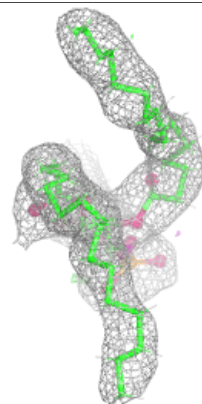
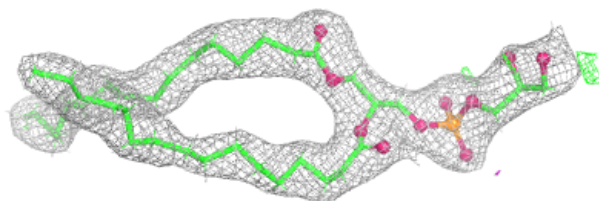
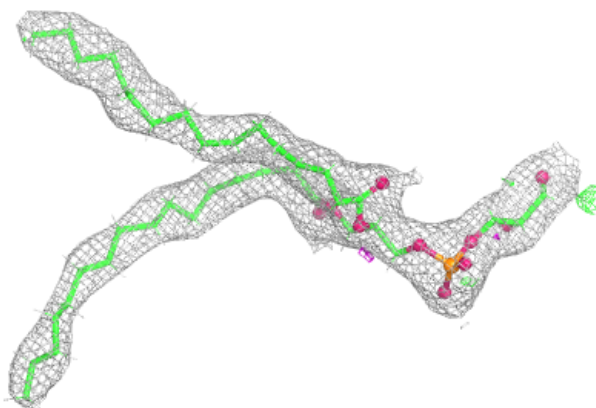


Electron density around CLA C 511:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

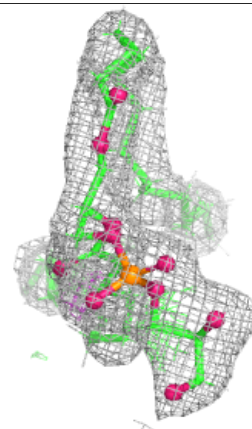
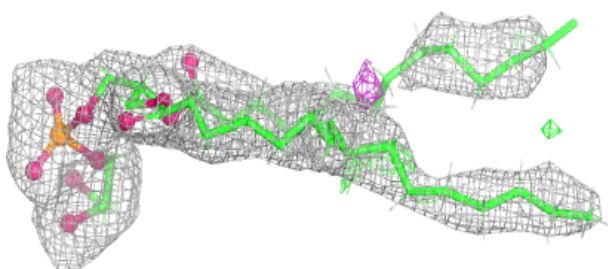
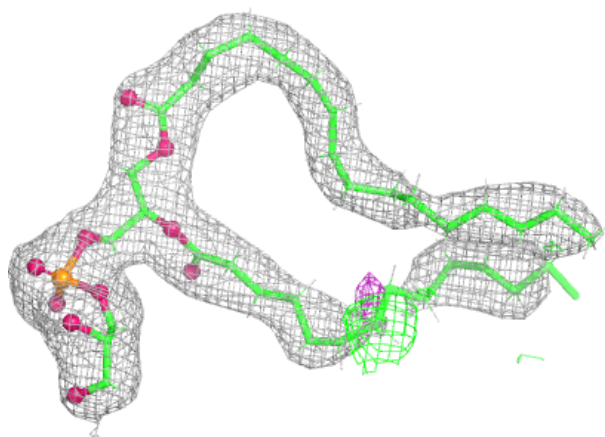
**Electron density around LHG D 410:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

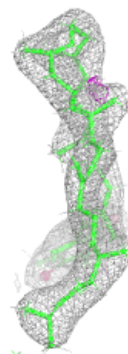
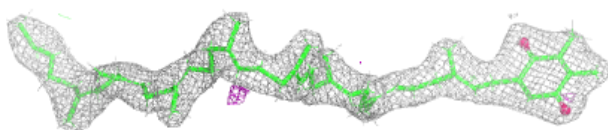
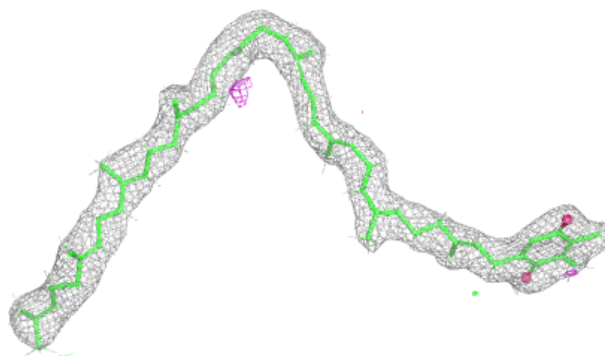


Electron density around LHG D 411:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

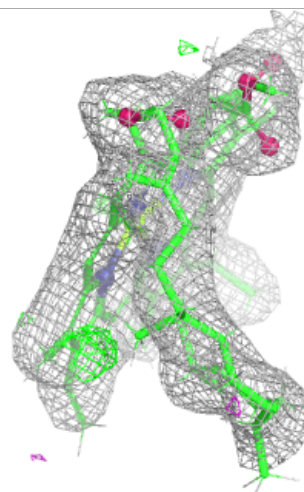
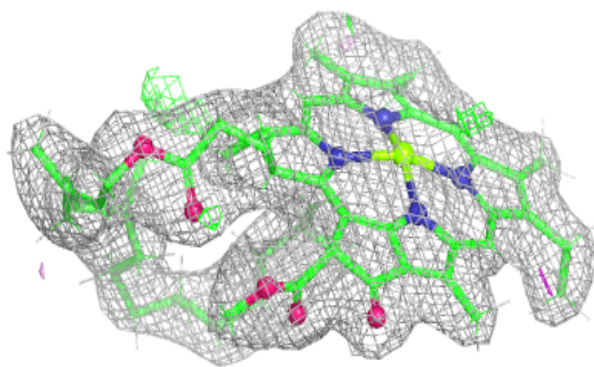
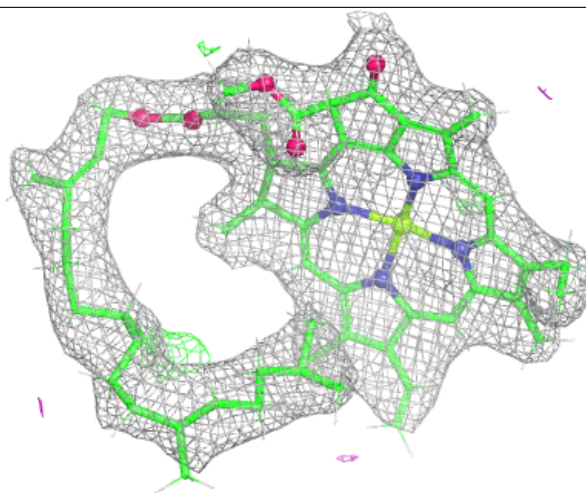
**Electron density around PL9 D 407:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



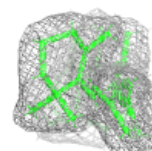
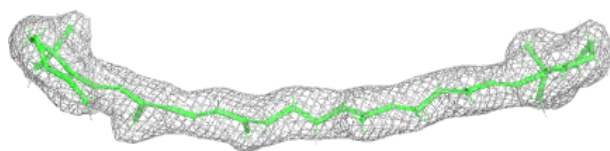
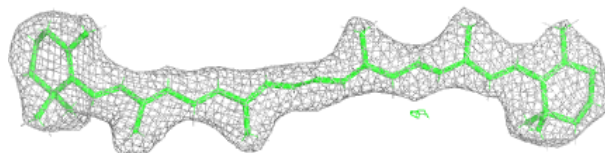
Electron density around CLA B 614:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

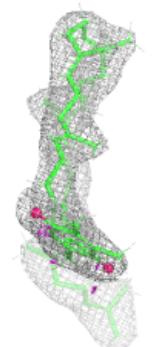
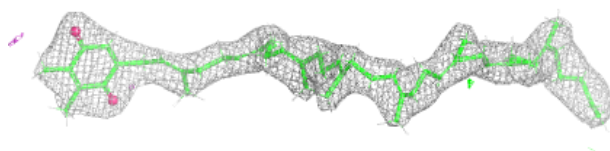
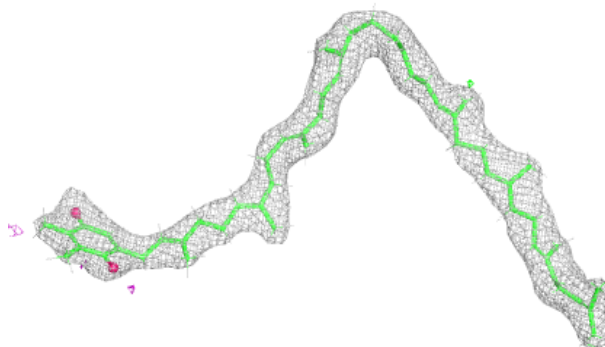


Electron density around BCR t 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

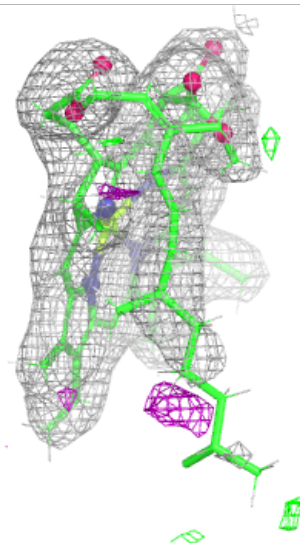
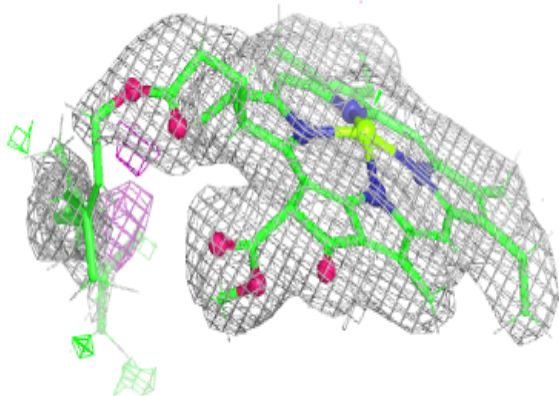
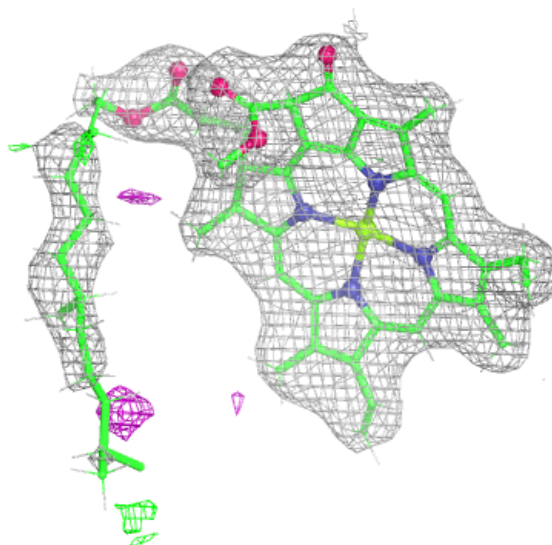
**Electron density around PL9 d 407:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



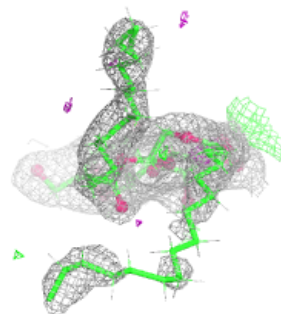
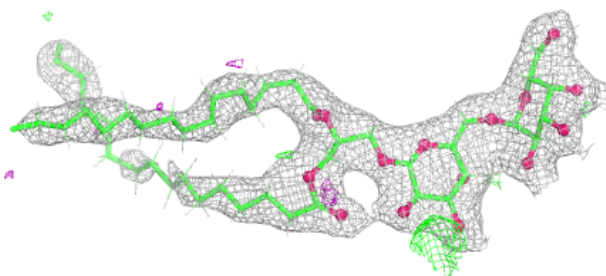
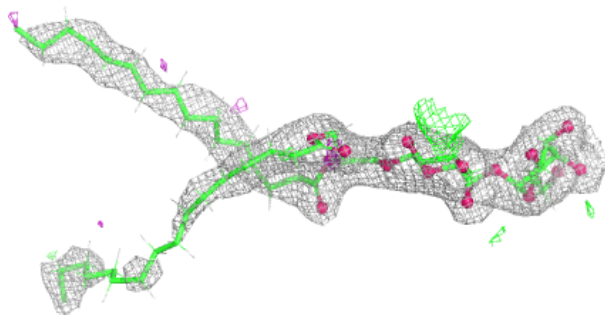
Electron density around CLA B 615:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

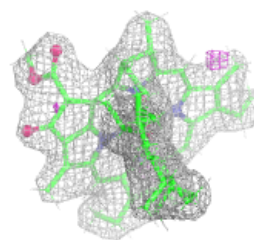
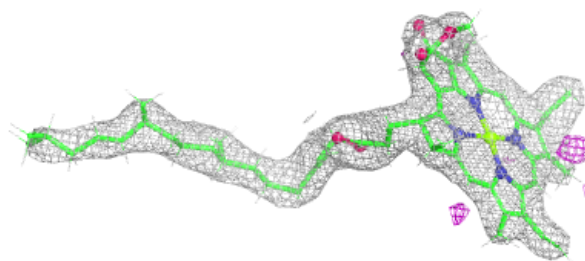
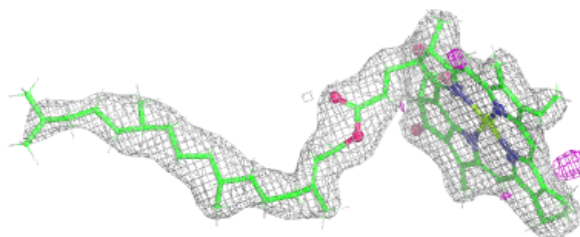


Electron density around DGD C 516:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

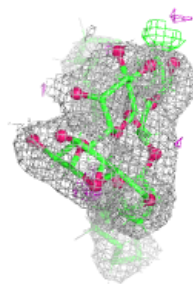
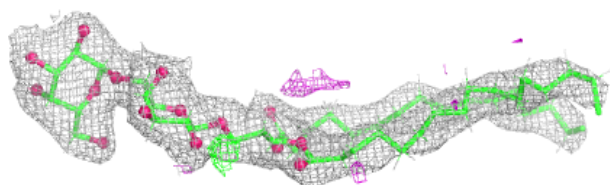
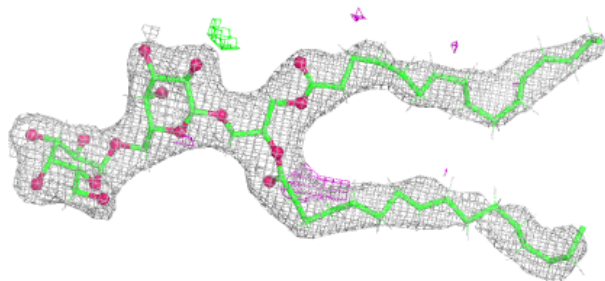
**Electron density around CLA C 502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

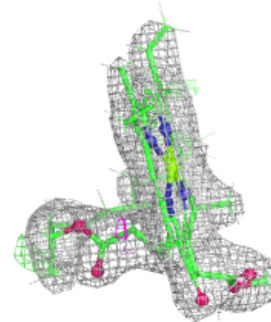
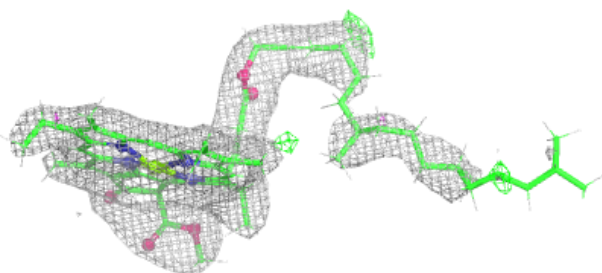
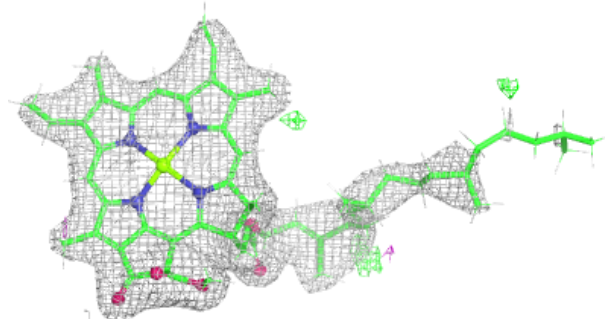


Electron density around DGD C 518:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

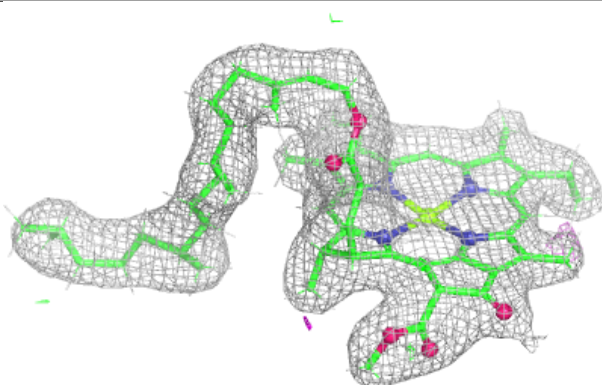
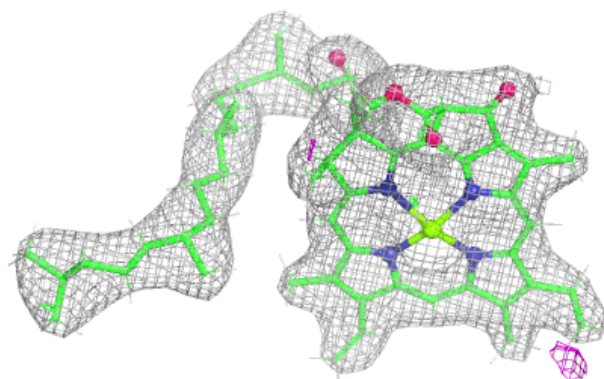
**Electron density around CLA a 403:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

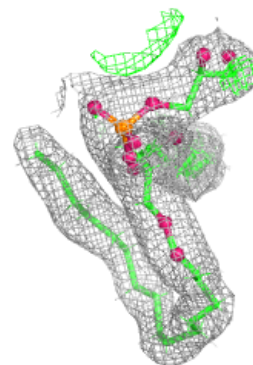
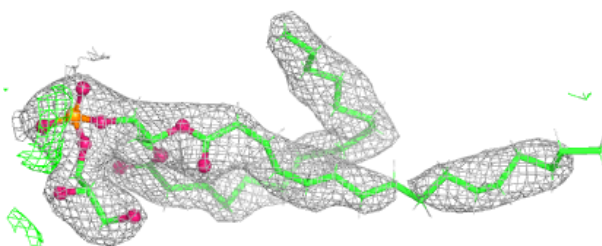
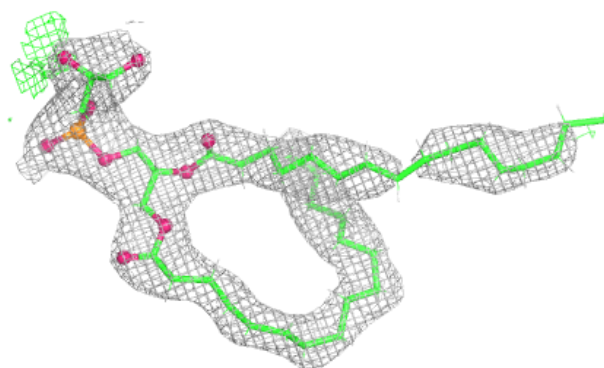


Electron density around CLA d 404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

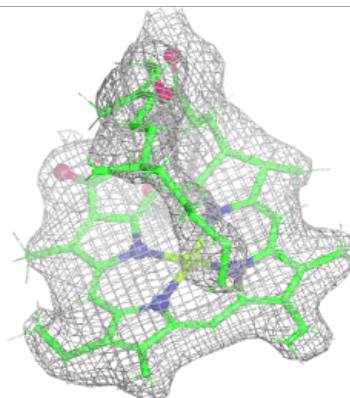
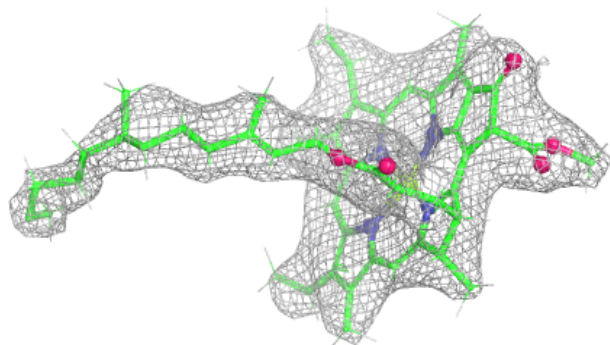
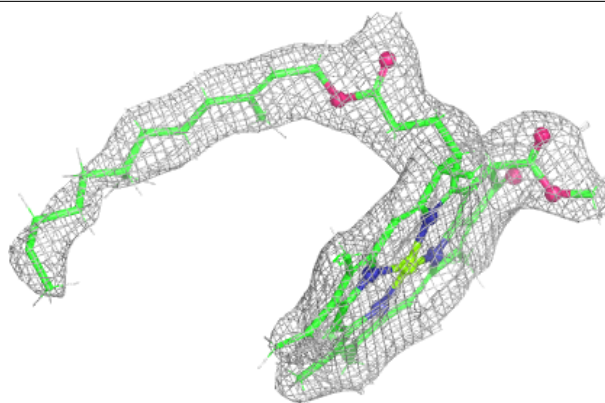
**Electron density around LHG D 413:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

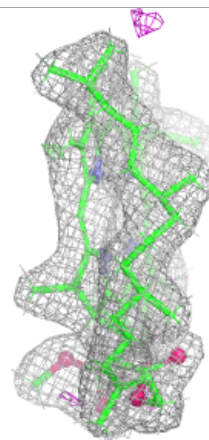
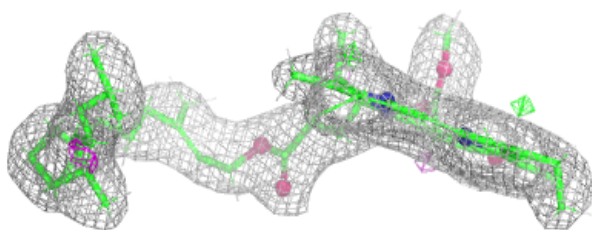
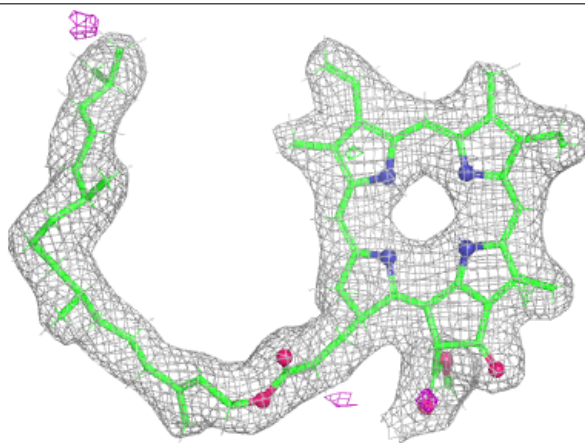


Electron density around CLA C 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

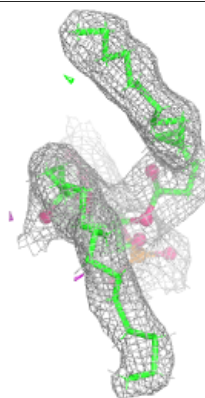
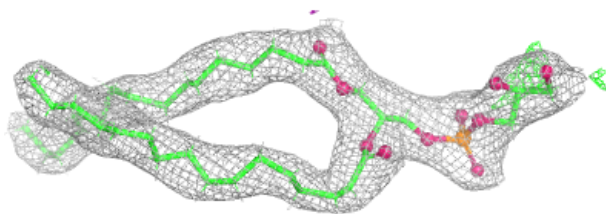
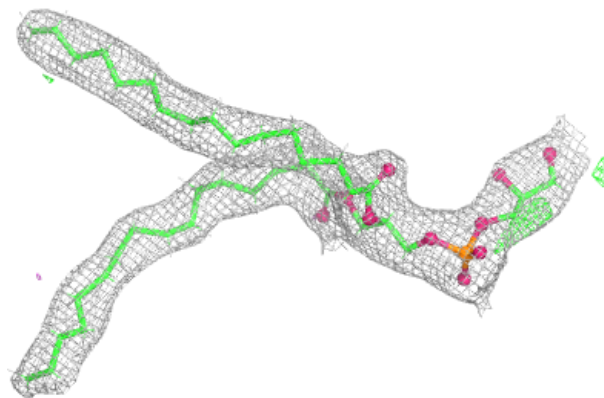
**Electron density around PHO A 404:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

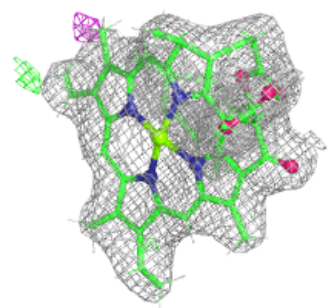
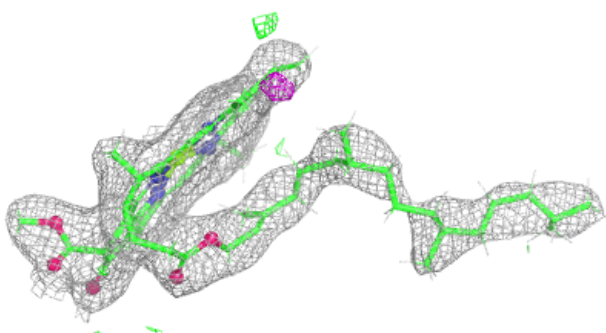
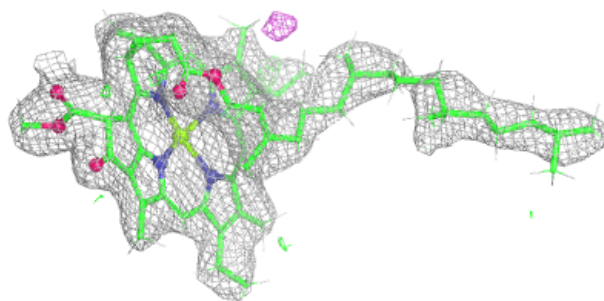


Electron density around LHG d 408:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

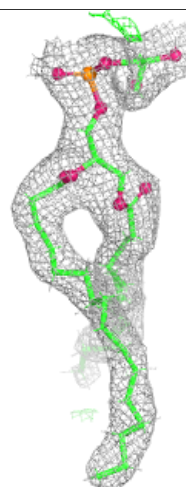
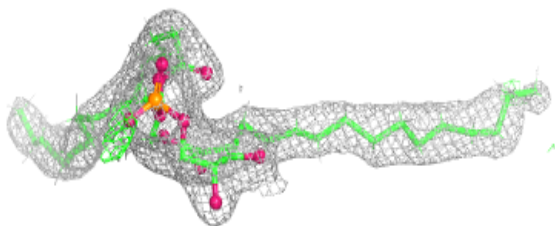
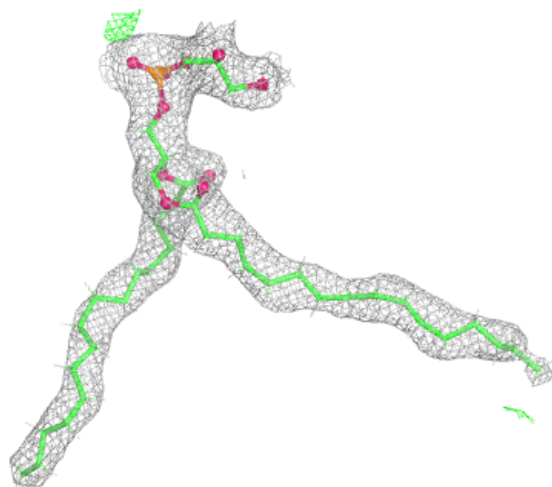
**Electron density around CLA C 505:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



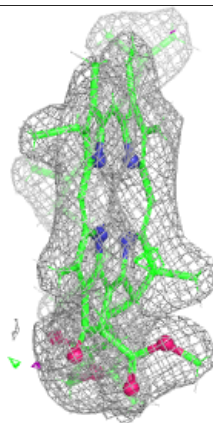
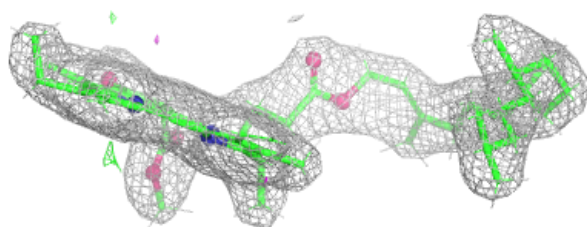
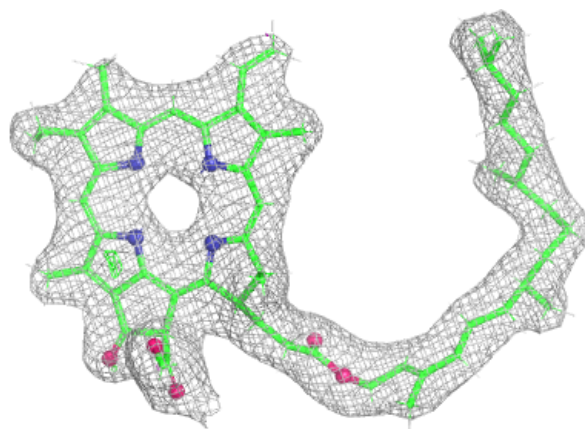
Electron density around LHG 1 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

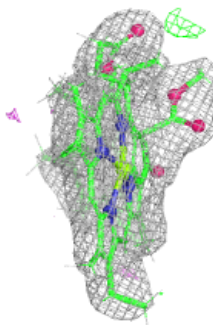
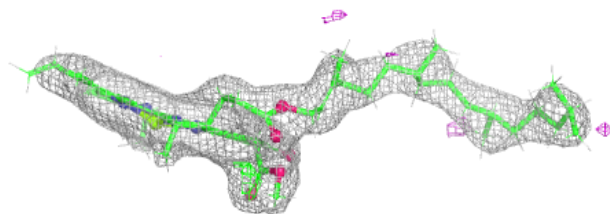
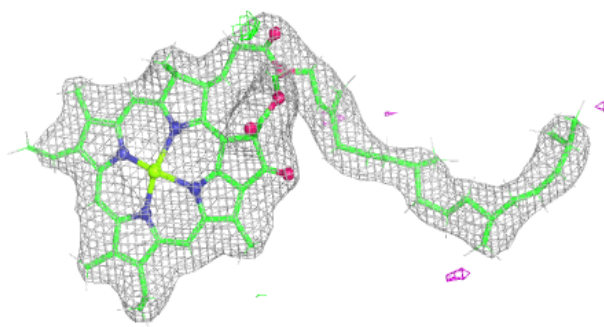


Electron density around PHO a 404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

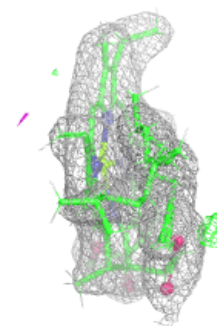
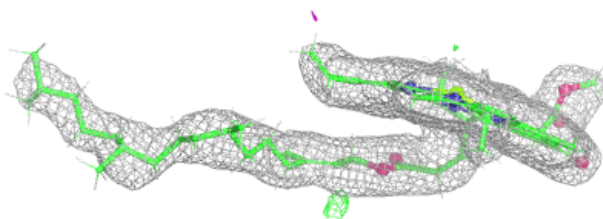
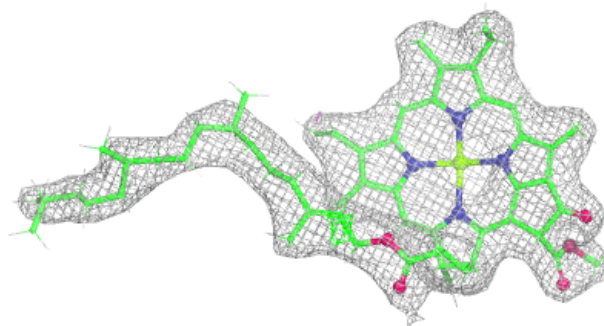
**Electron density around CLA b 602:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

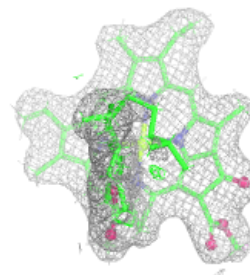
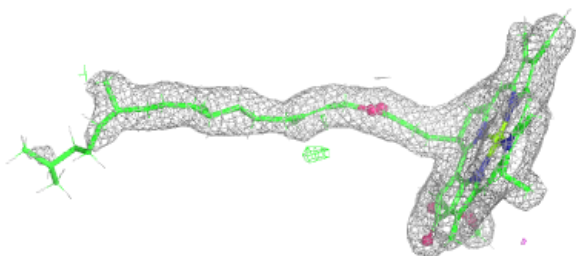
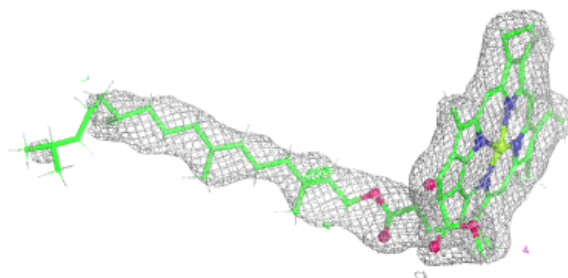


Electron density around CLA b 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

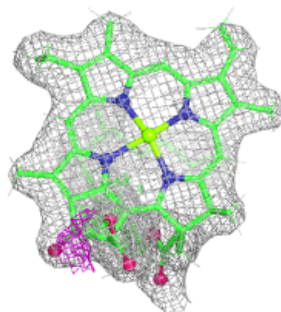
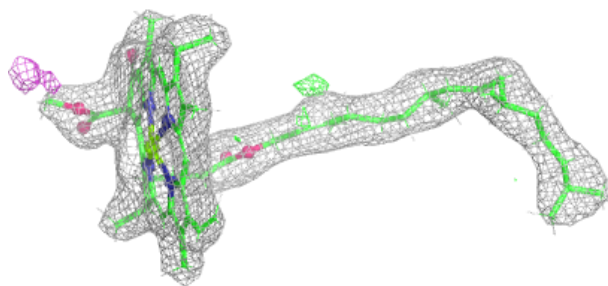
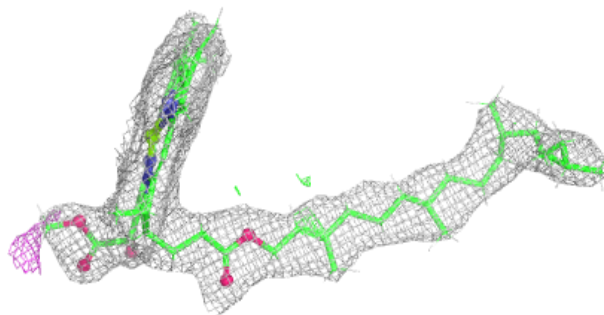
**Electron density around CLA b 604:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

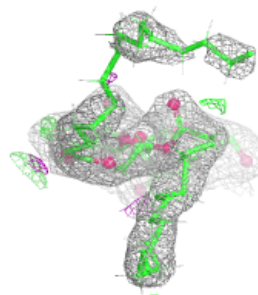
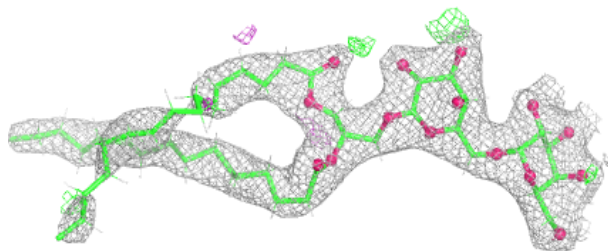
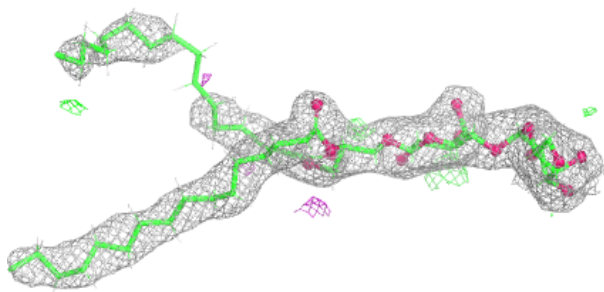


Electron density around CLA b 605:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

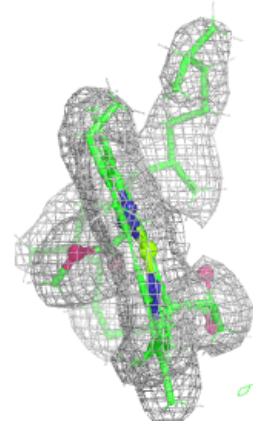
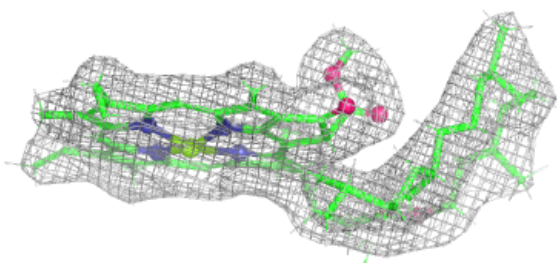
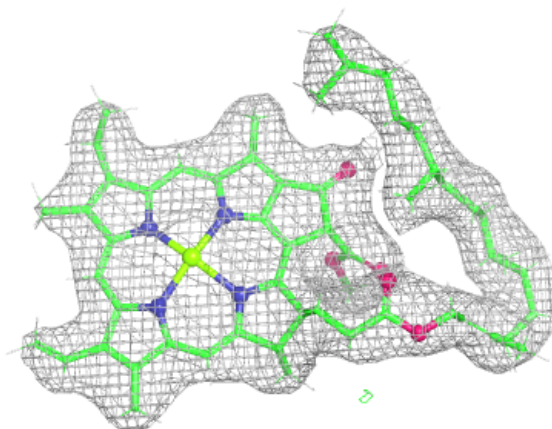
**Electron density around DGD c 515:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

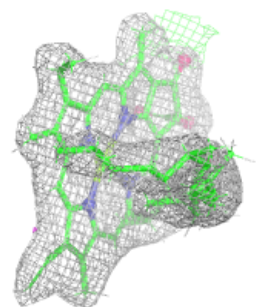
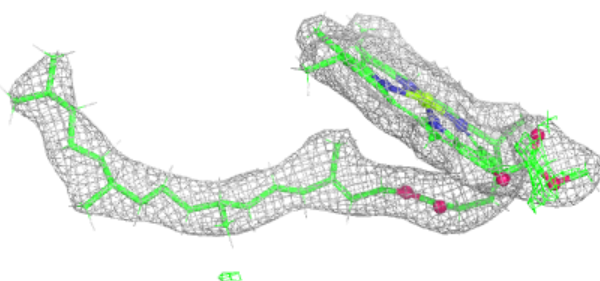
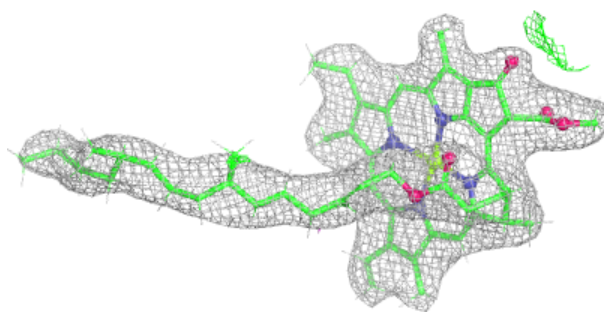


Electron density around CLA B 609:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

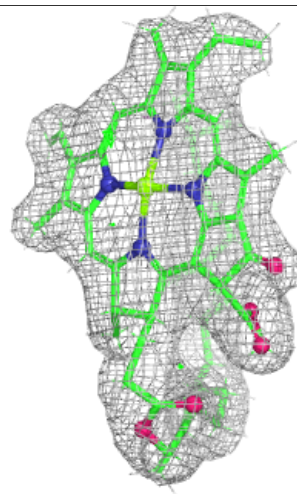
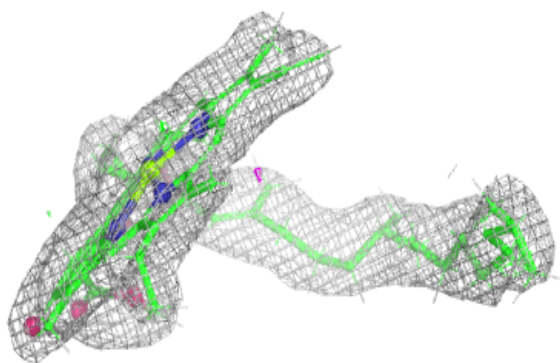
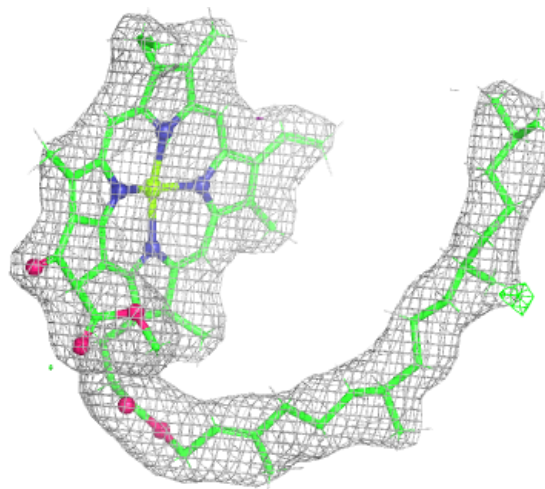
**Electron density around CLA b 608:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



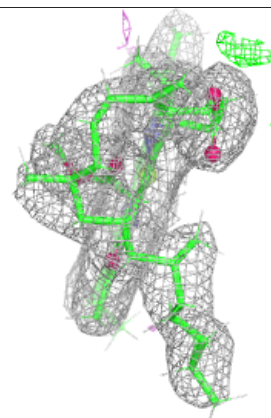
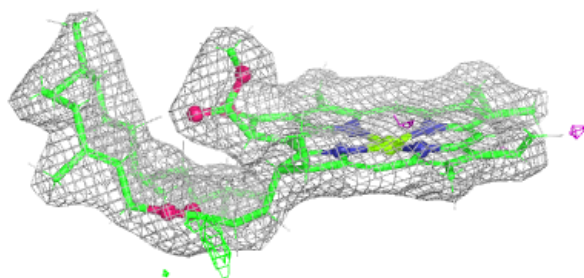
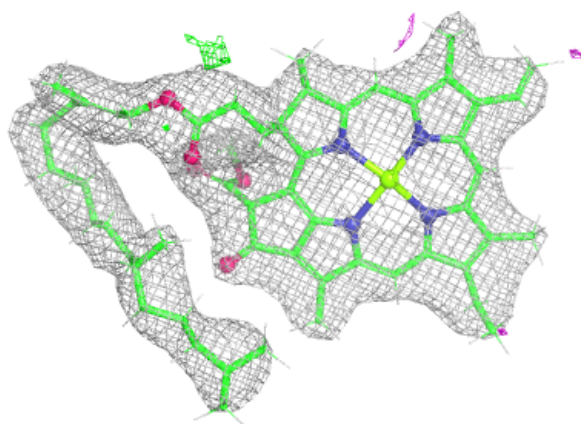
Electron density around CLA C 507:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



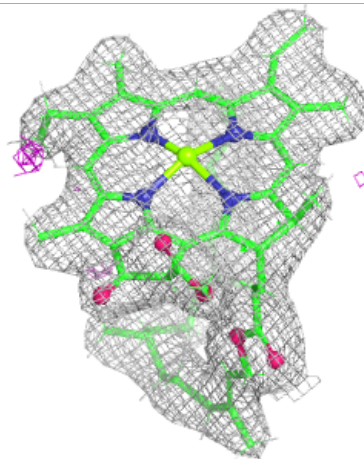
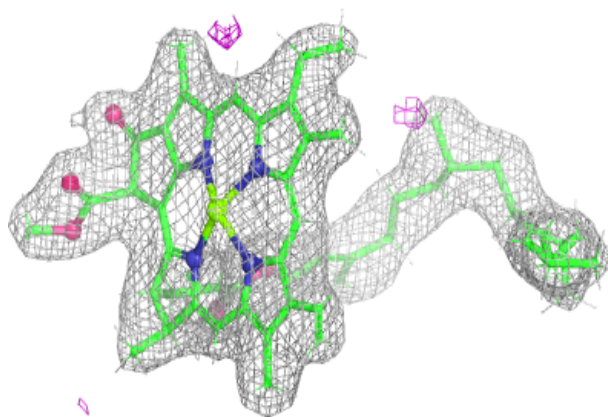
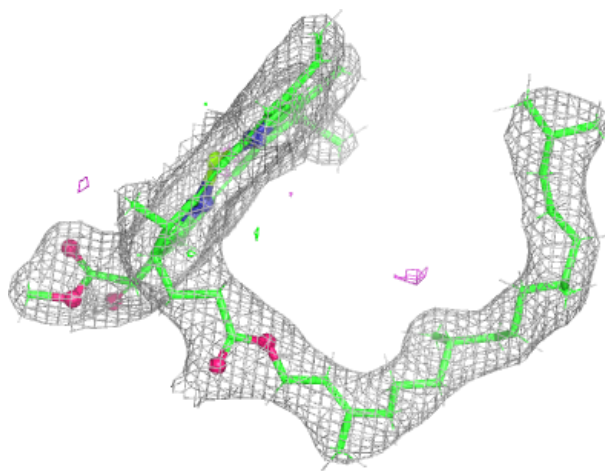
Electron density around CLA b 610:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



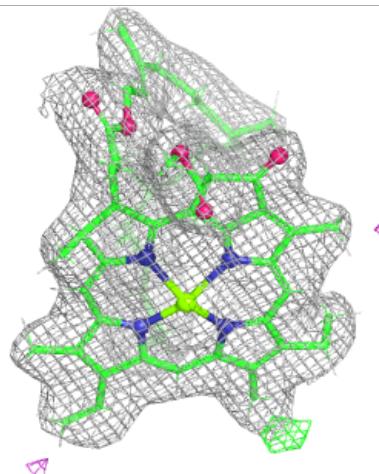
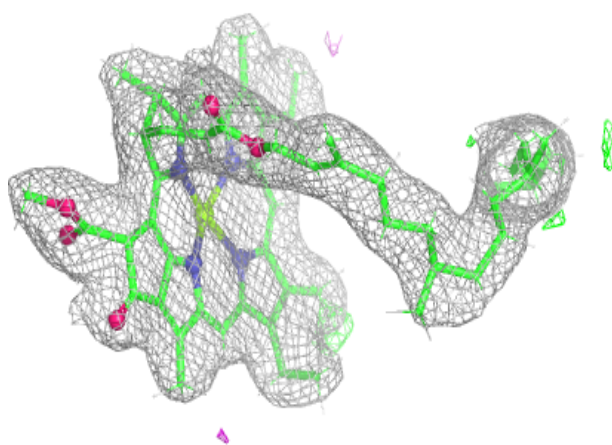
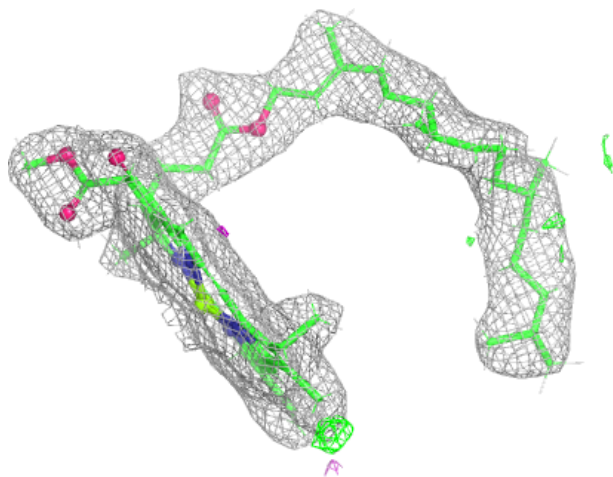
Electron density around CLA b 611:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



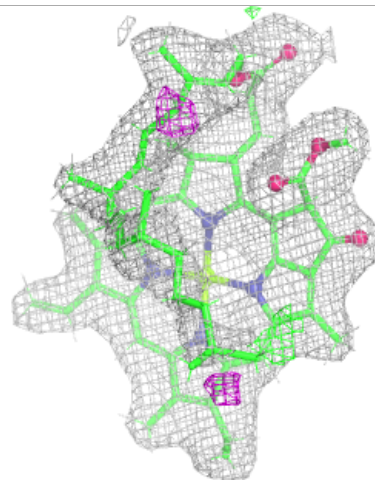
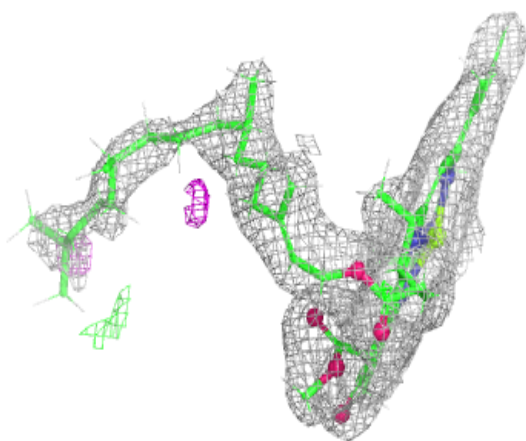
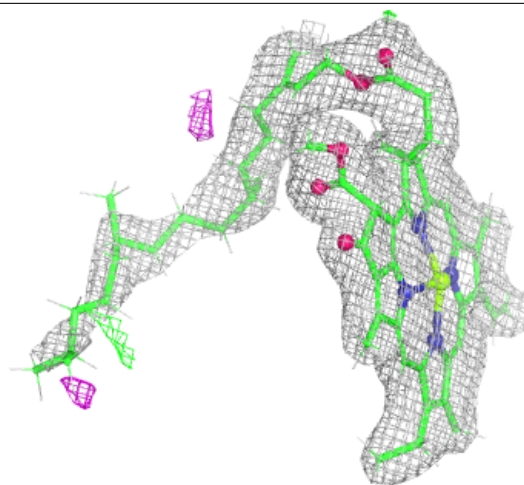
Electron density around CLA B 610:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



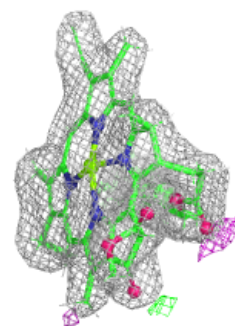
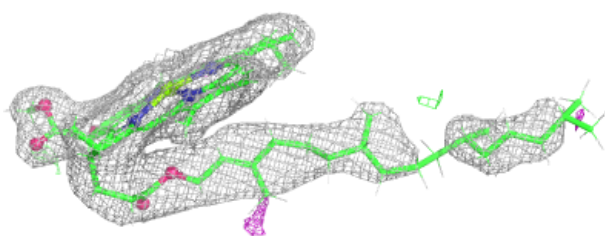
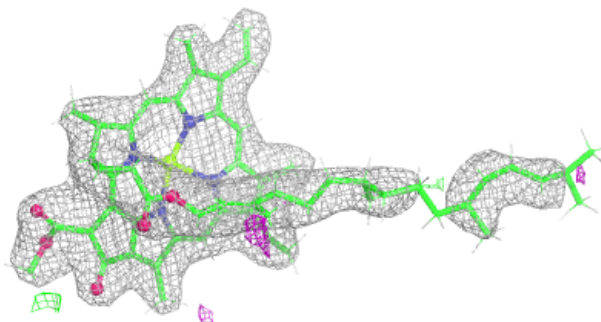
Electron density around CLA b 613:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

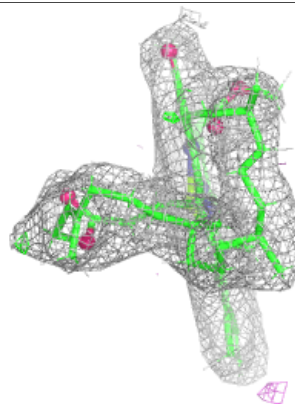
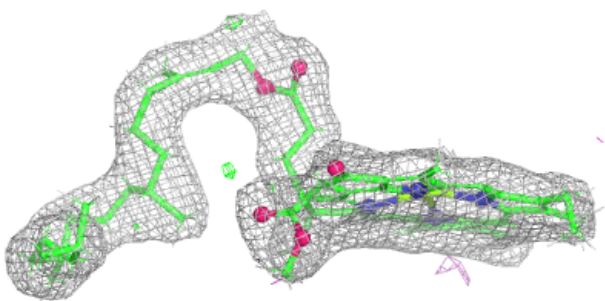
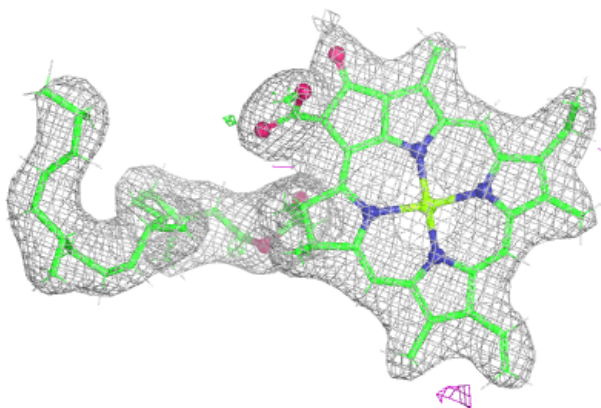


Electron density around CLA b 614:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

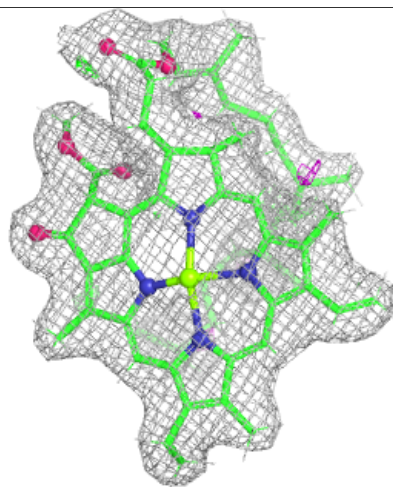
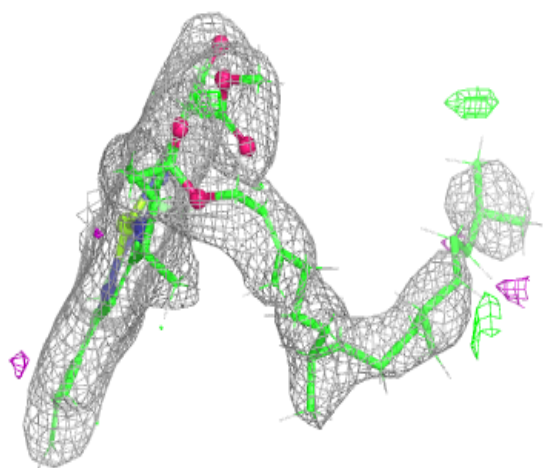
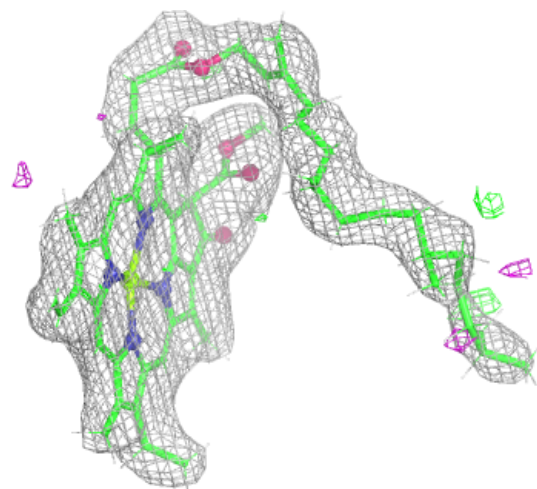
**Electron density around CLA B 611:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



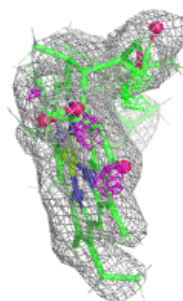
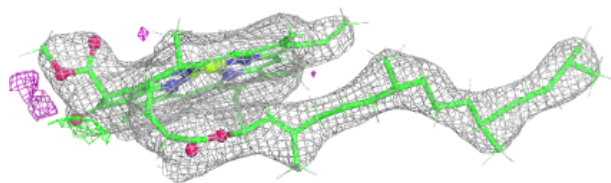
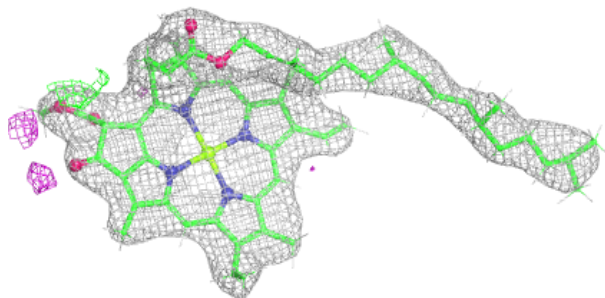
Electron density around CLA B 612:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

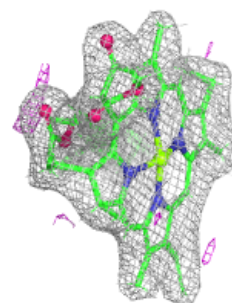
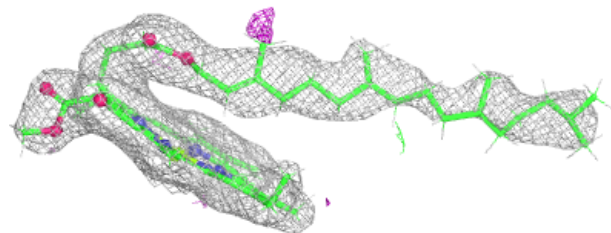
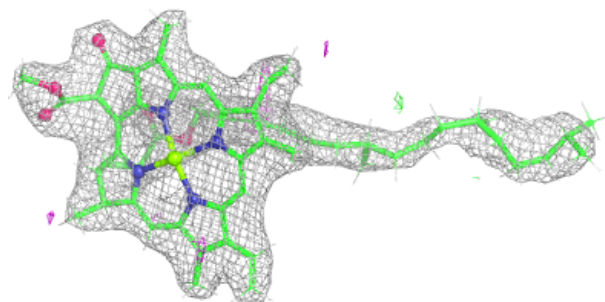


Electron density around CLA c 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

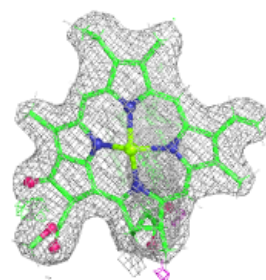
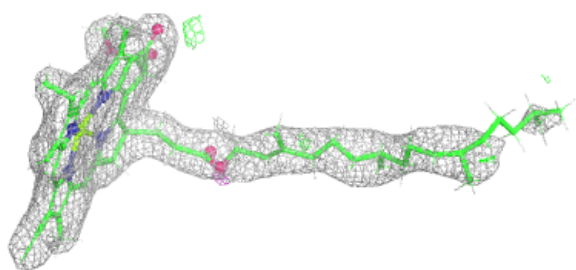
**Electron density around CLA B 613:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

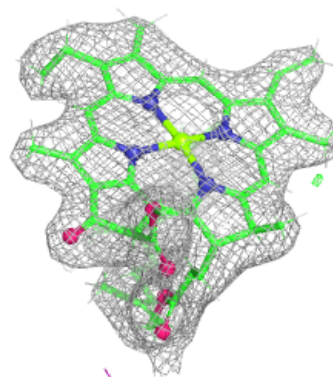
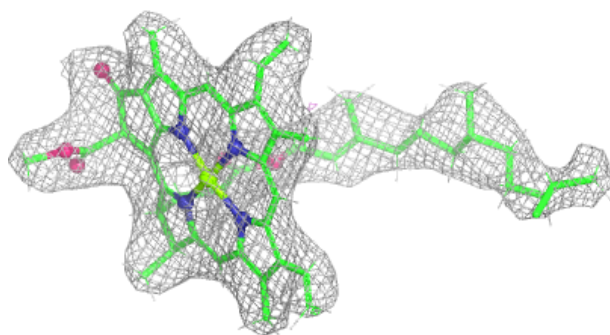
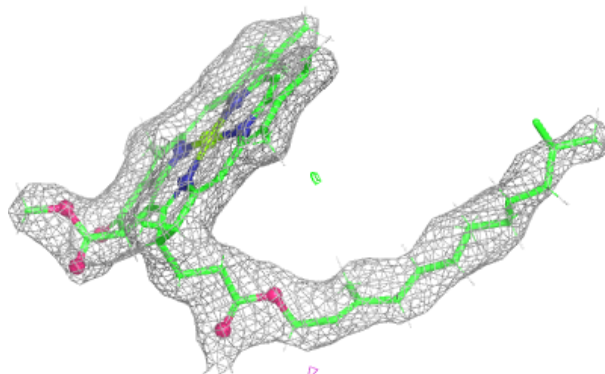


Electron density around CLA B 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

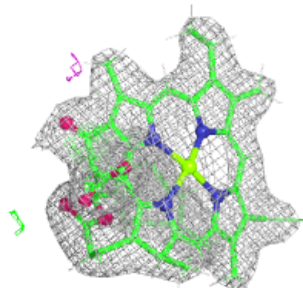
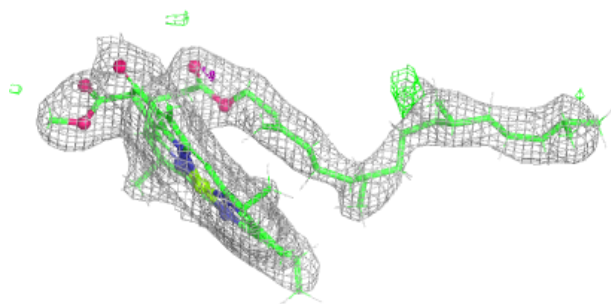
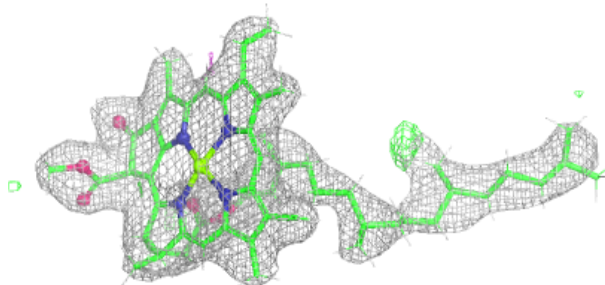
**Electron density around CLA c 504:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

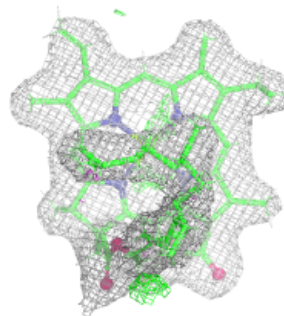
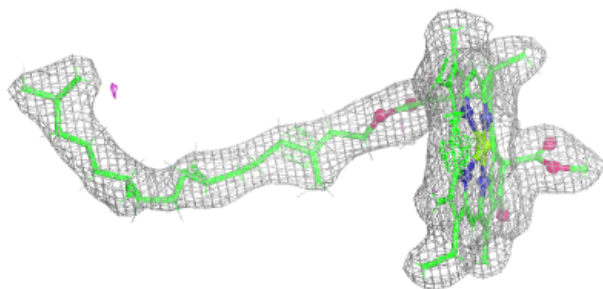
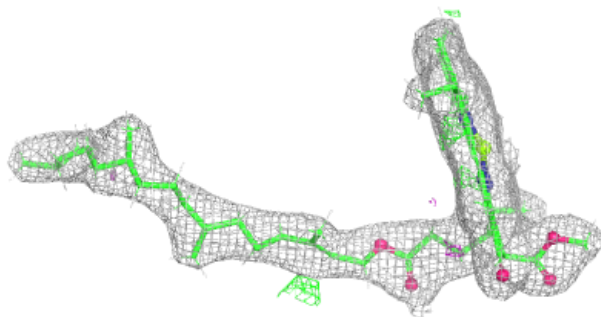


Electron density around CLA c 505:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

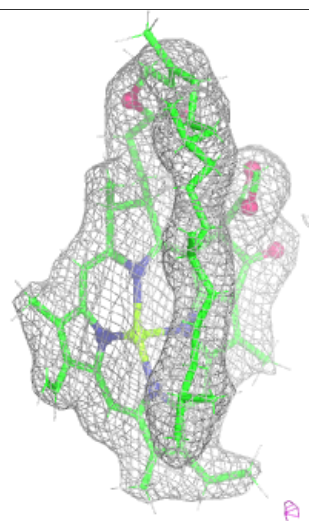
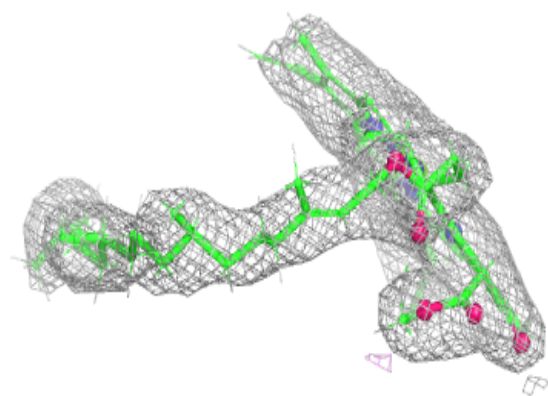
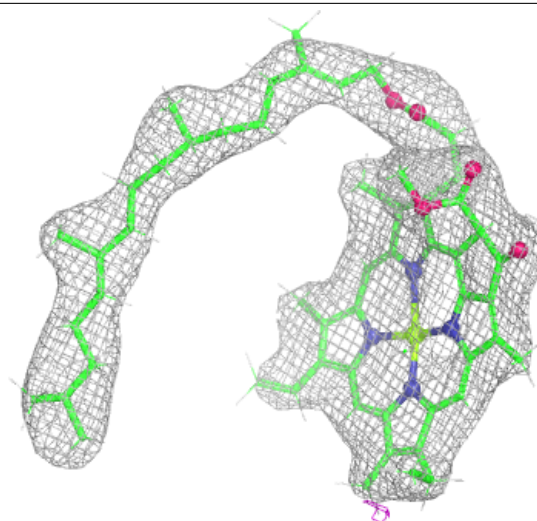
**Electron density around CLA B 604:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



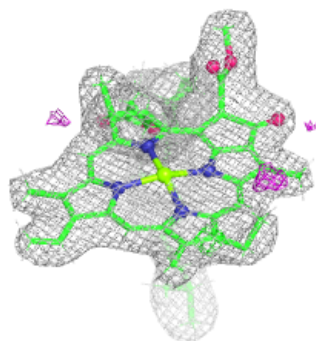
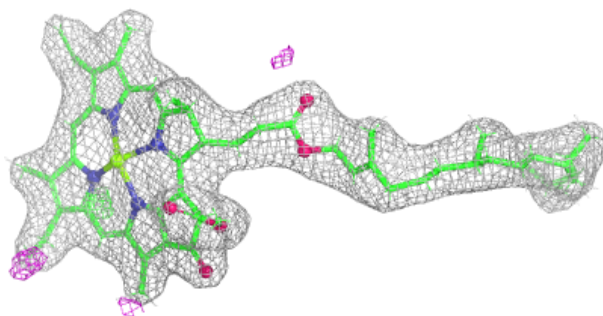
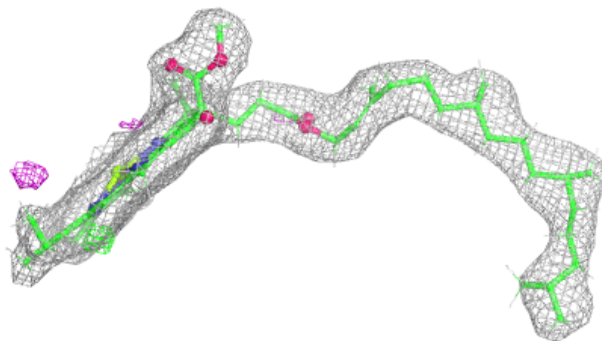
Electron density around CLA c 507:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

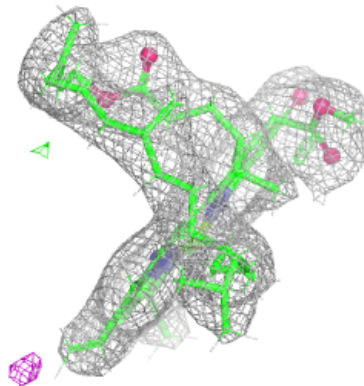
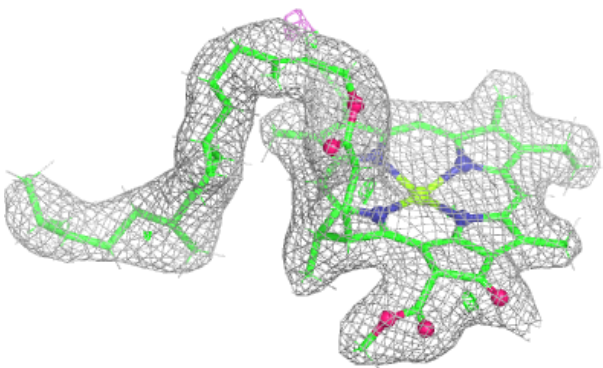
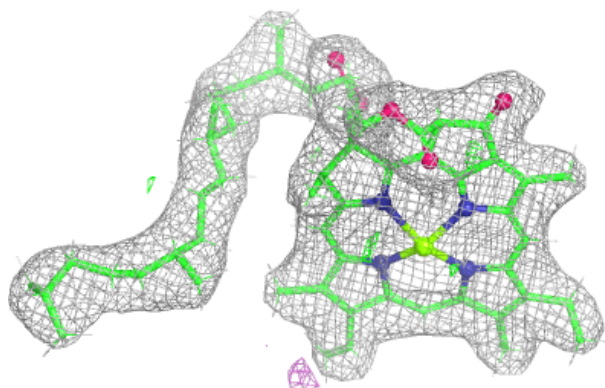


Electron density around CLA D 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

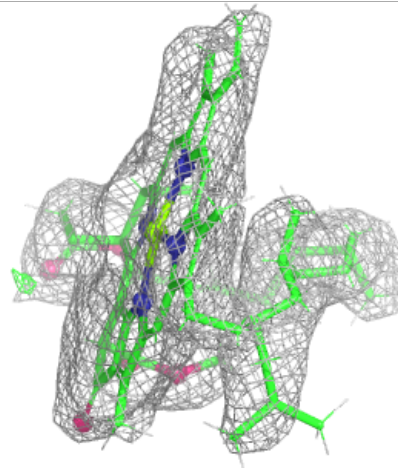
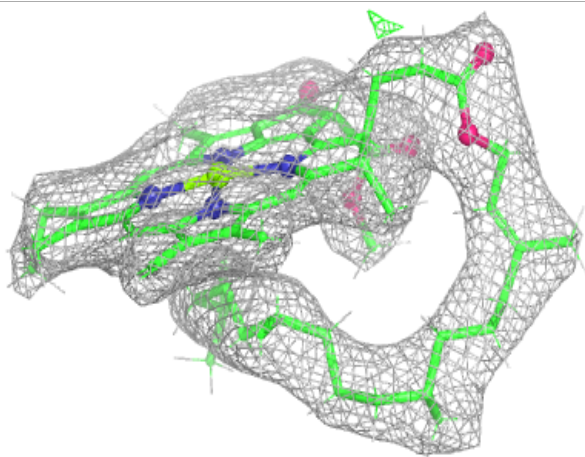
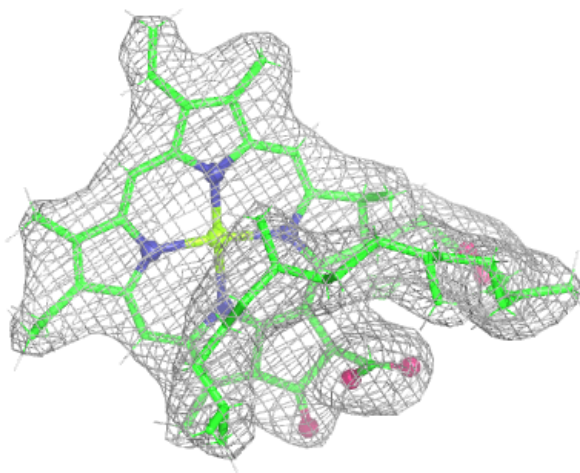
**Electron density around CLA D 404:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



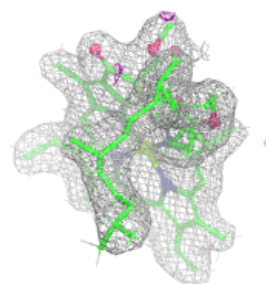
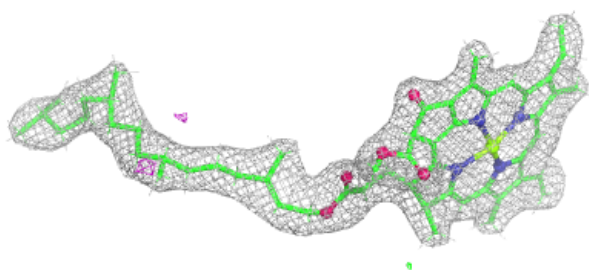
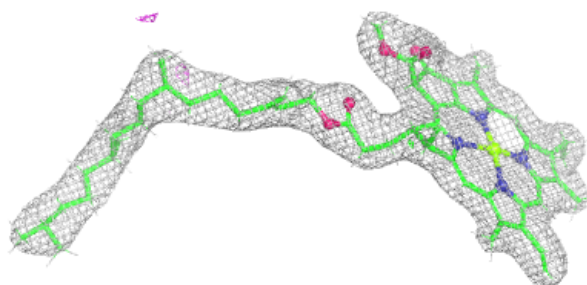
Electron density around CLA c 510:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

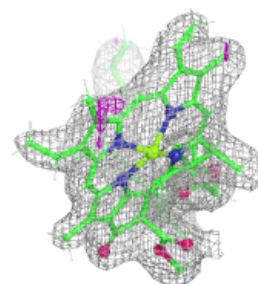
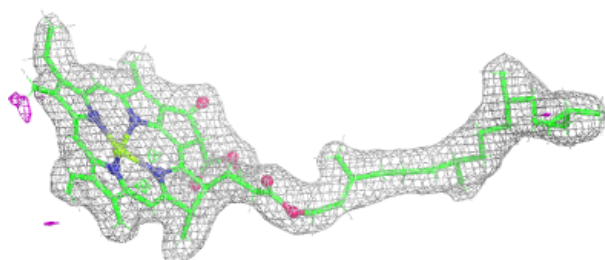
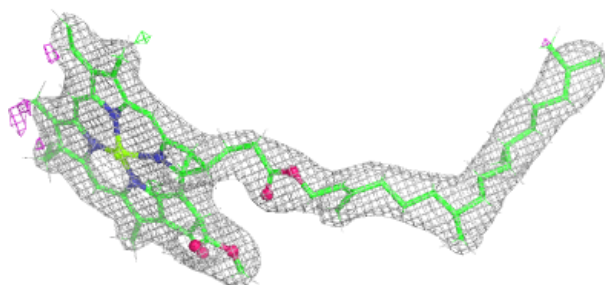


Electron density around CLA A 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

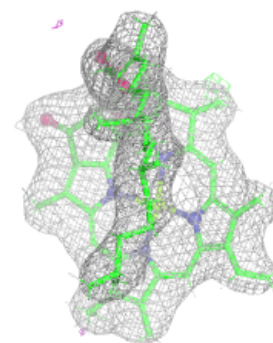
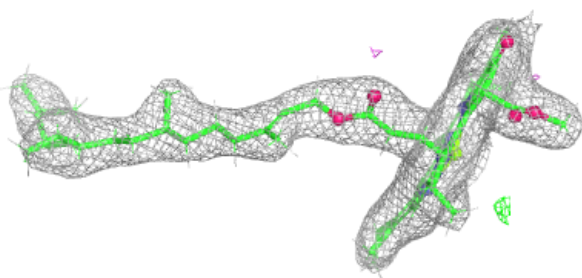
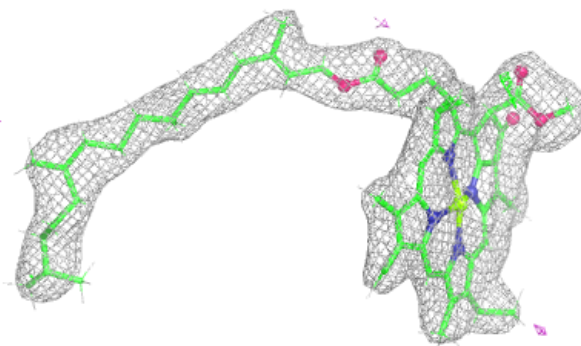
**Electron density around CLA a 402:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

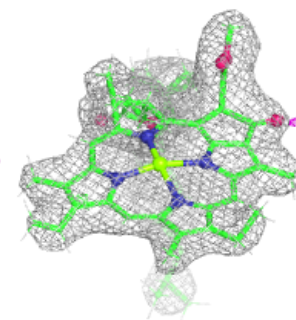
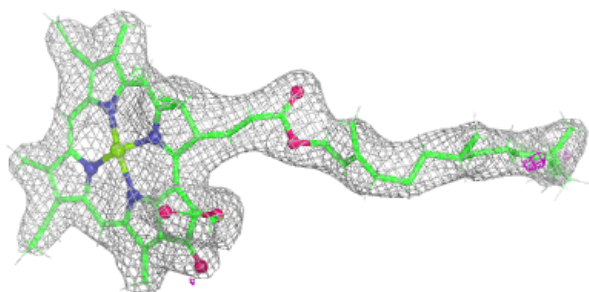
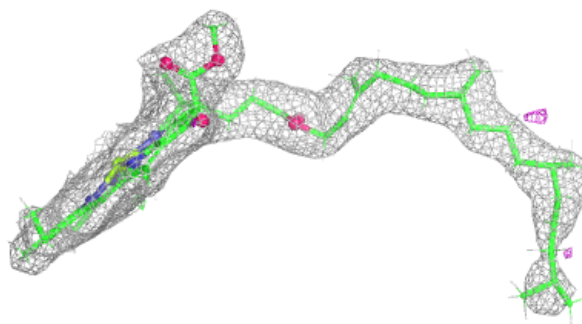


Electron density around CLA B 608:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

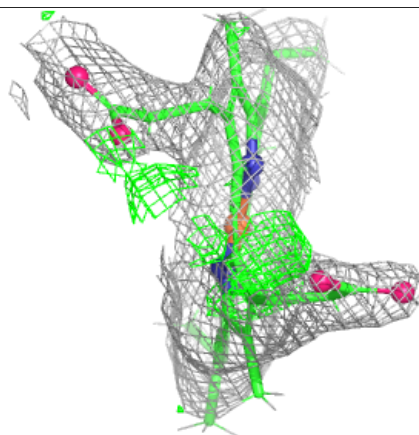
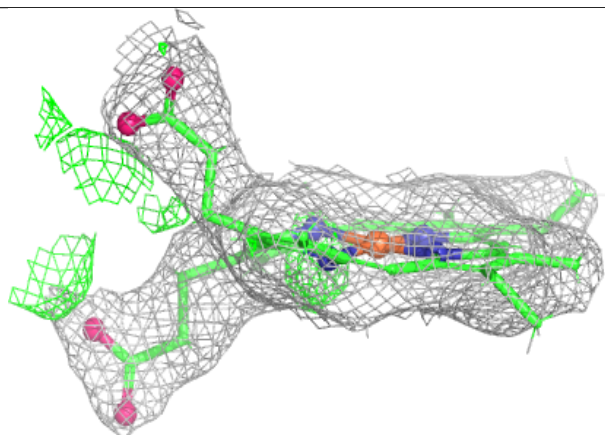
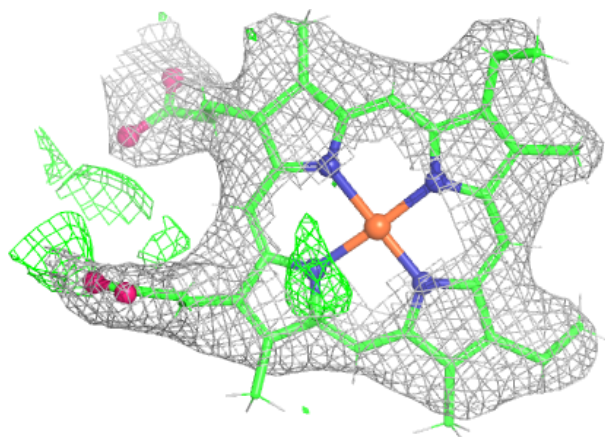
**Electron density around CLA d 403:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

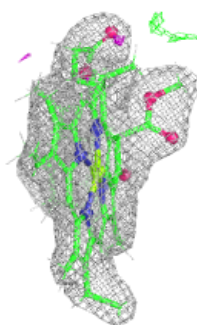
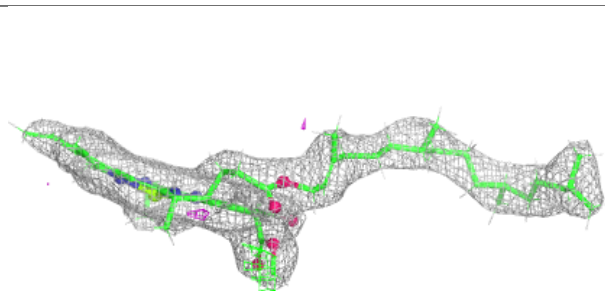
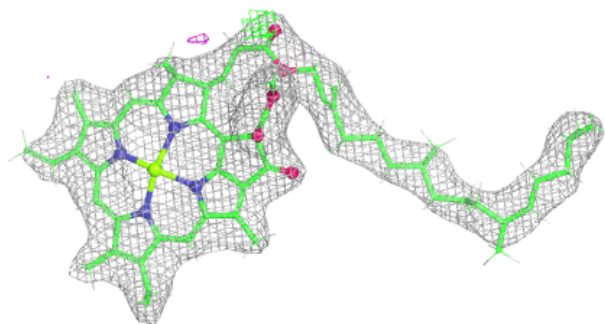


Electron density around HEC f 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

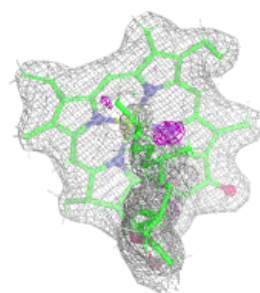
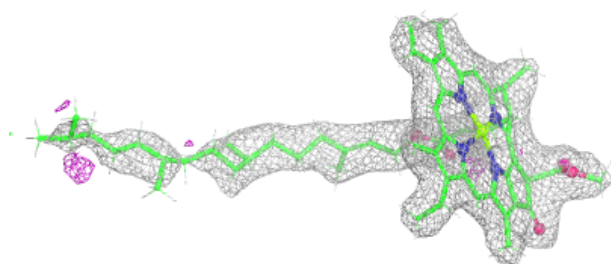
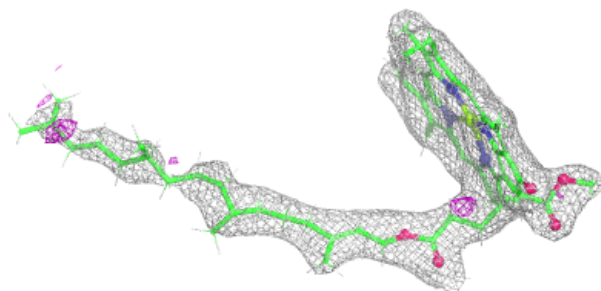
**Electron density around CLA B 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

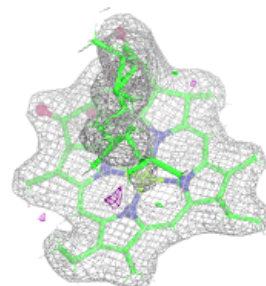
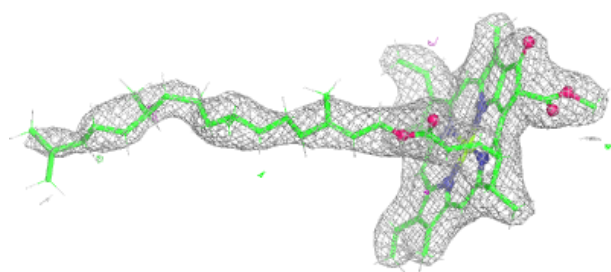
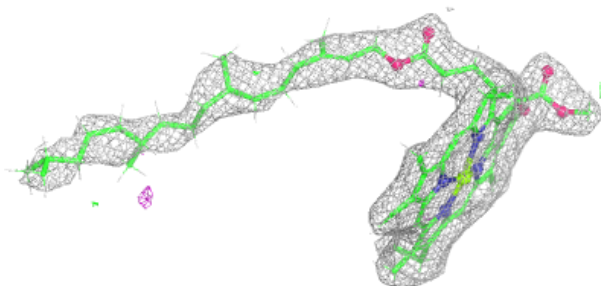


Electron density around CLA b 607:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

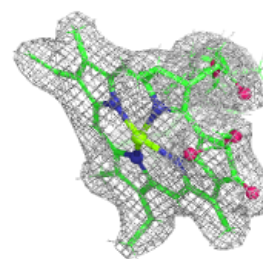
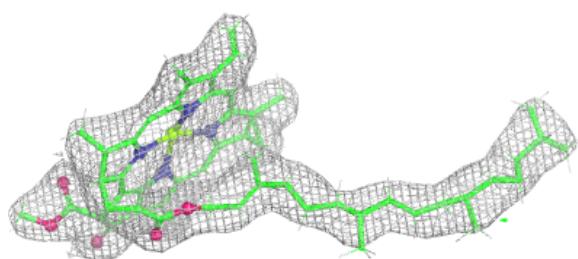
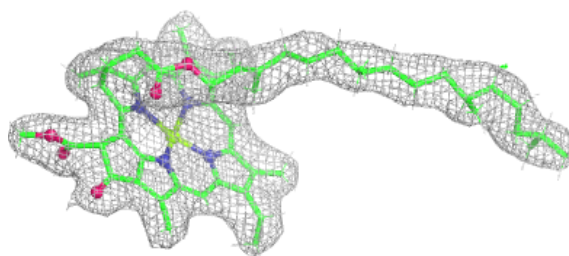
**Electron density around CLA B 606:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

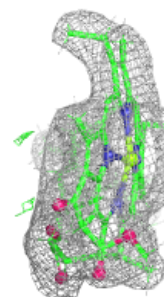
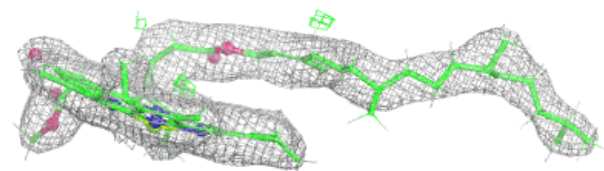
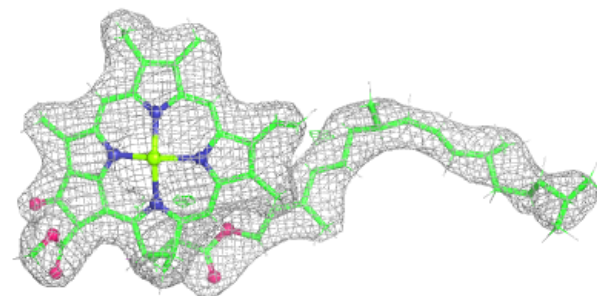


Electron density around CLA B 607:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

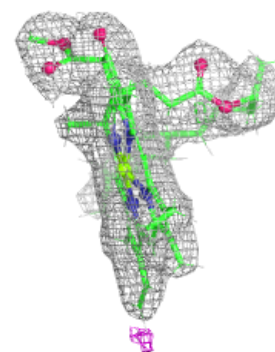
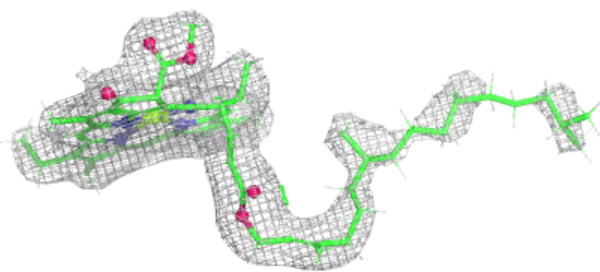
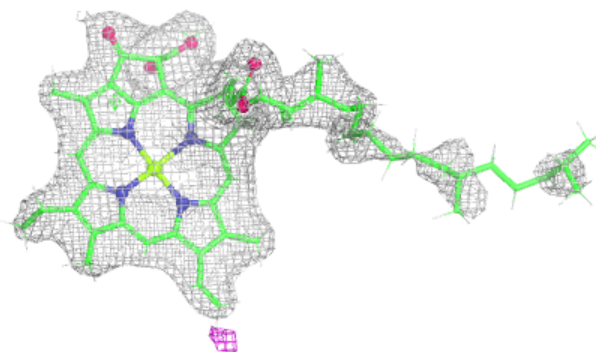
**Electron density around CLA B 602:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



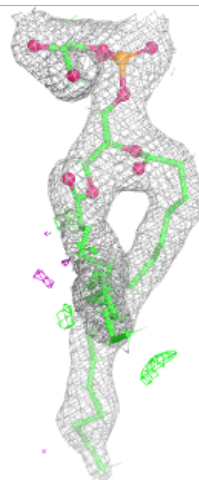
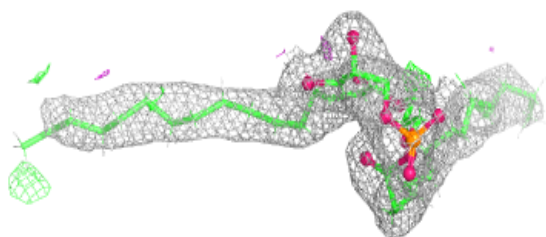
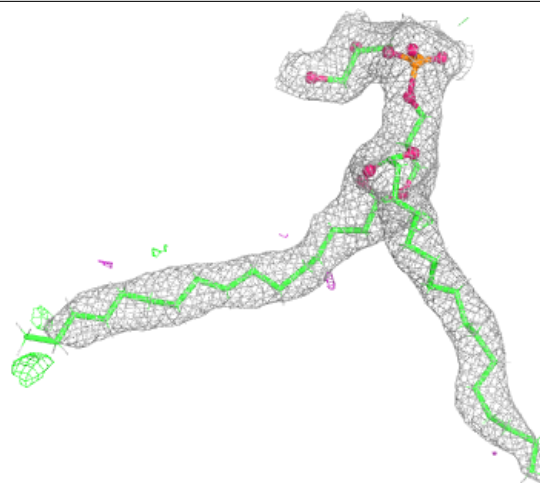
Electron density around CLA A 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



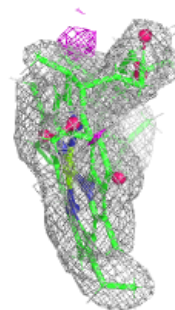
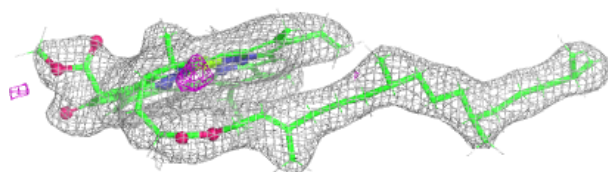
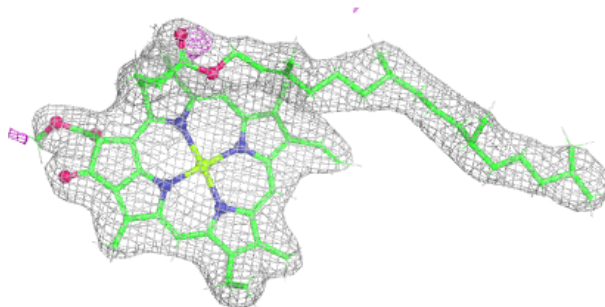
Electron density around LHG L 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

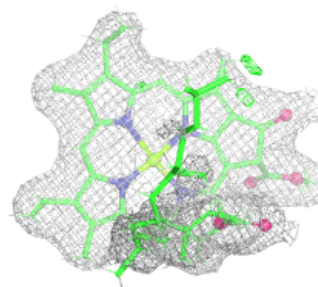
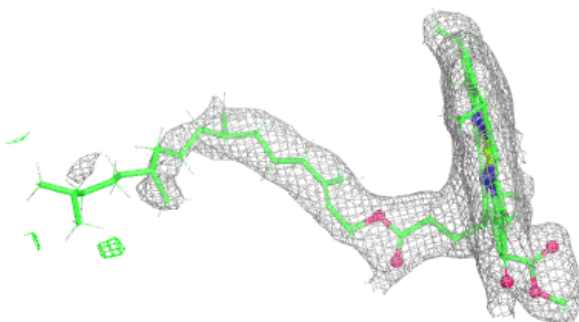
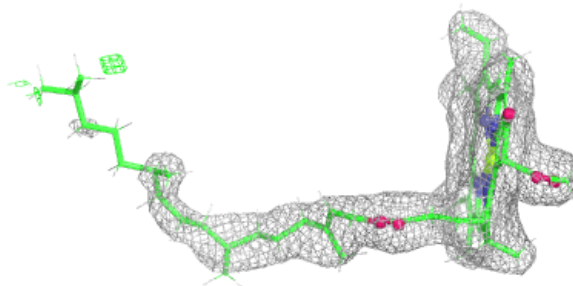


Electron density around CLA C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

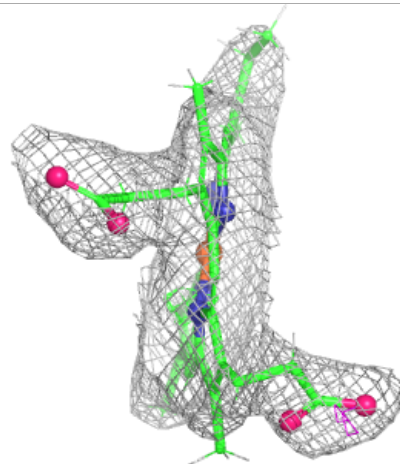
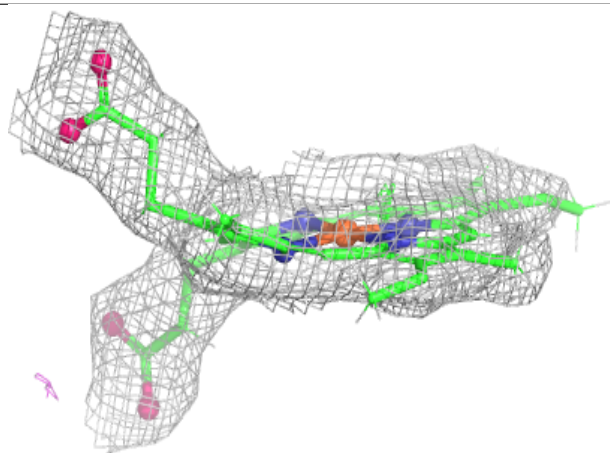
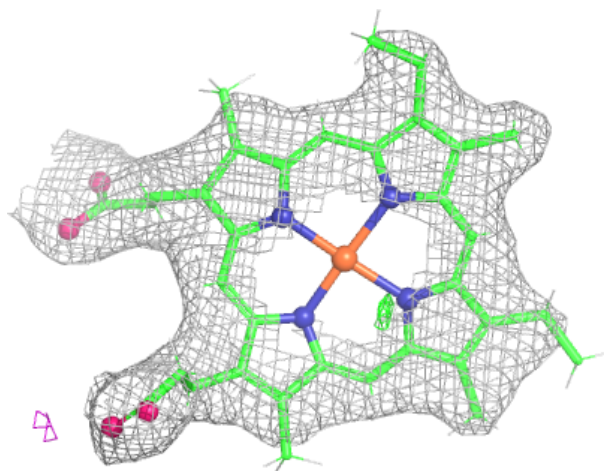
**Electron density around CLA D 405:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



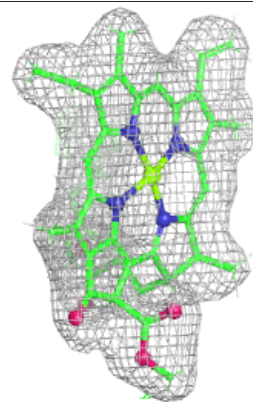
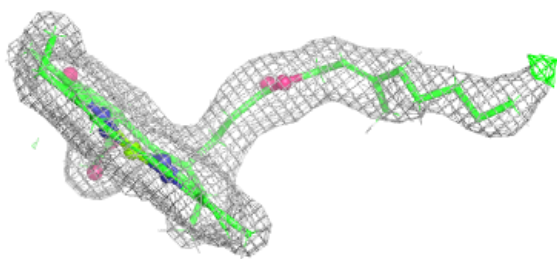
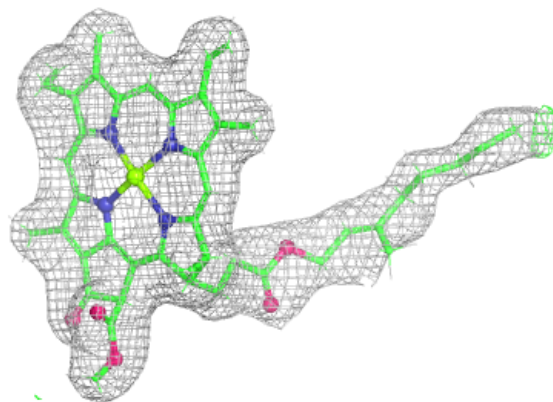
Electron density around HEC F 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



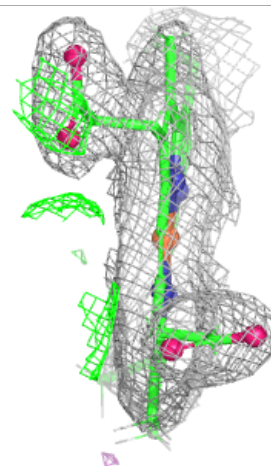
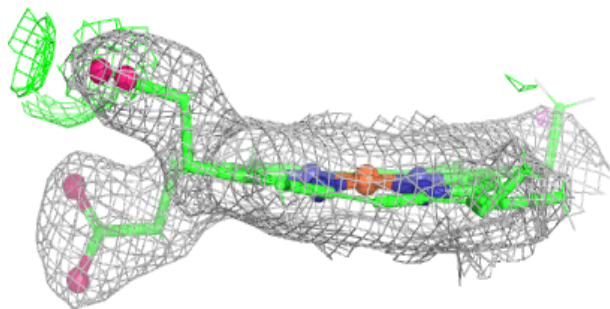
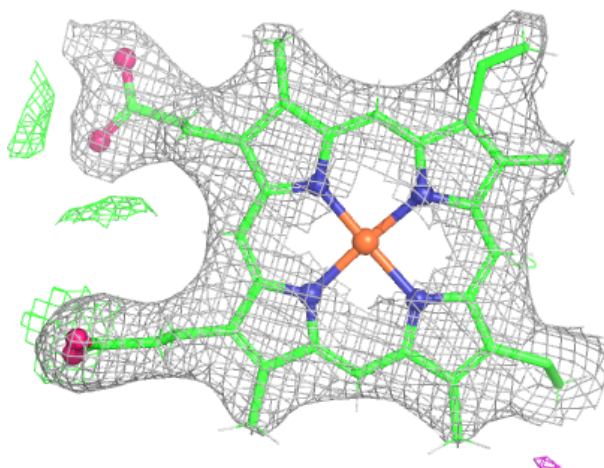
Electron density around CLA A 405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



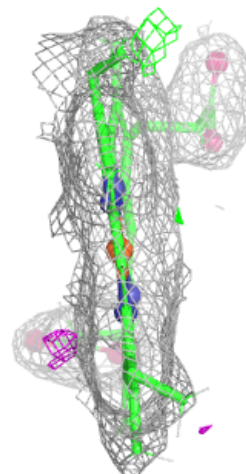
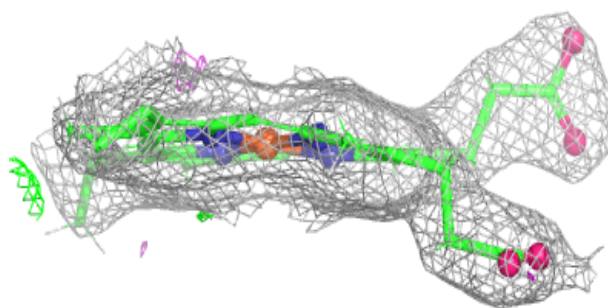
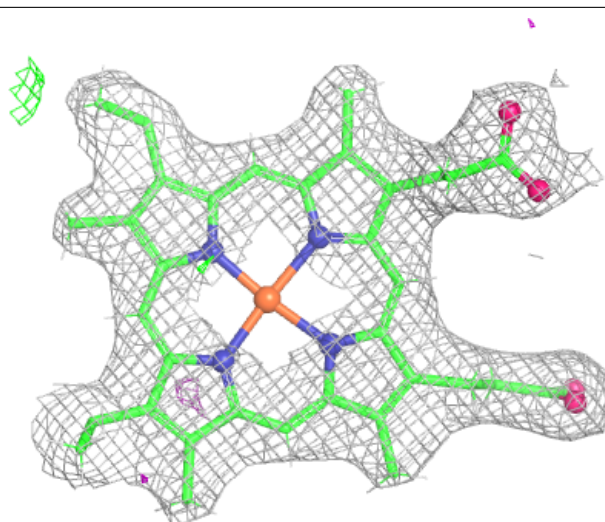
Electron density around HEC v 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC V 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.